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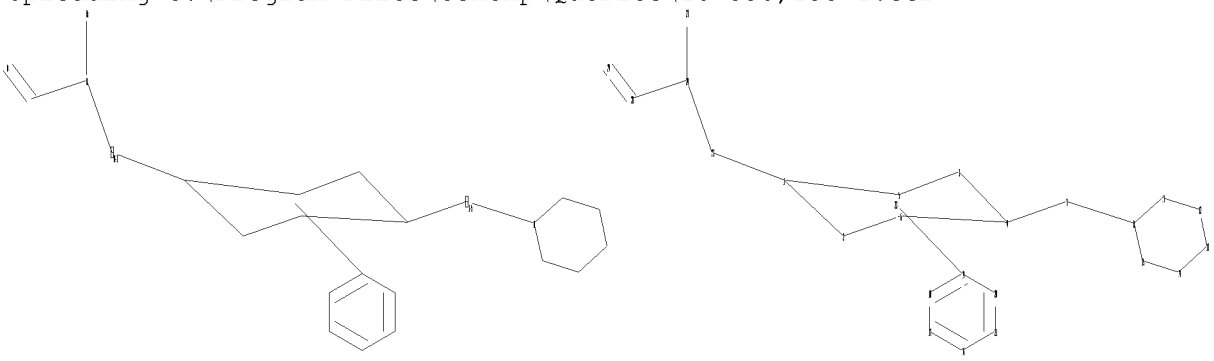

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ring nodes :
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1-23 4-7 7-8 23-24 24-27 24-28 28-29
ring bonds :
1-2 1-5 2-6 3-4 3-5 4-6 8-11 8-15 11-12 12-13 13-14 14-15 16-17 16-21
17-18 18-19 19-20 20-21
exact/norm bonds :
1-2 1-5 2-6 3-4 3-5 4-6 7-8 8-11 8-15 11-12 12-13 13-14 14-15 23-24
24-27 24-28 28-29
exact bonds :
1-23 4-7
normalized bonds :
16-17 16-21 17-18 18-19 19-20 20-21

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS
24:CLASS 27:CLASS 28:CLASS 29:CLASS

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L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:25:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    22962 TO ITERATE

  8.7% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       450169 TO   468311
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:25:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   462831 TO ITERATE

100.0% PROCESSED   462831 ITERATIONS                              39 ANSWERS
SEARCH TIME: 00.00.12

L3           39 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               178.82     179.03

FILE 'CAPLUS' ENTERED AT 10:26:11 ON 22 OCT 2008
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FILE COVERS 1907 - 22 Oct 2008 VOL 149 ISS 17
FILE LAST UPDATED: 21 Oct 2008 (20081021/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4 1 L3

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YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y

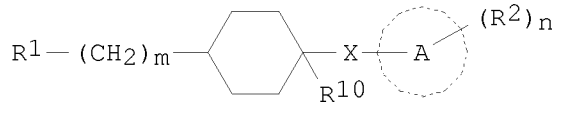
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:531360 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 141:88873
TITLE: Preparation of heterocyclylalkyl substituted cyclohexyl compounds as CCR5 antagonists
INVENTOR(S): Duan, Maosheng; Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054581	A2	20040701	WO 2003-US39732	20031212
WO 2004054581	A3	20050203		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003297048	A1	20040709	AU 2003-297048	20031212
EP 1569647	A2	20050907	EP 2003-813435	20031212
EP 1569647	B1	20080820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006514646	T	20060511	JP 2004-560857	20031212
AT 405269	T	20080915	AT 2003-813435	20031212
US 20060122166	A1	20060608	US 2005-538135	20050609

PRIORITY APPLN. INFO.: US 2002-433552P P 20021213
WO 2003-US39732 W 20031212

OTHER SOURCE(S): MARPAT 141:88873

GI



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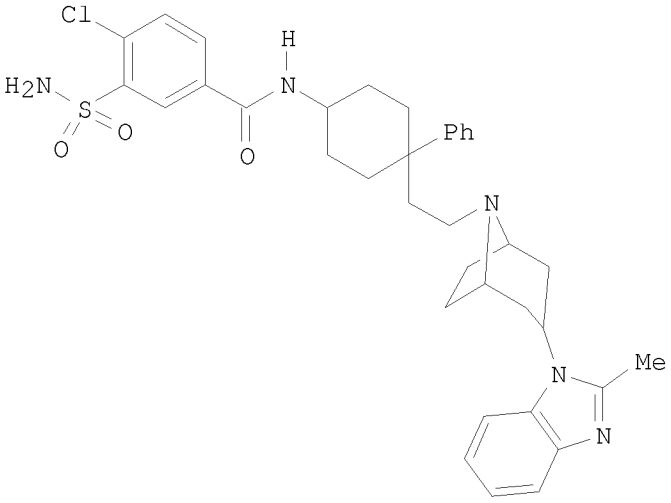

II

AB Title compds. I [R1 = (un)substituted saturated, partially saturated, or aromatic 4-7
monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from O, P, S or N, optionally attached through alkylene chain, substituted-amine, -amide, etc.; R2 = OH, halogen (un)substituted-alkyl, -alkoxy, -aryl, -heteroaryl, -cycloalkyl, etc., optionally two adjacent R2s taken together form a fused, saturated, partially saturated or aromatic 5-6 membered ring having 0-3 heteroatoms selected from O, P, S, or N, or two geminal R2s optionally taken together from a spiro, saturated, partially saturated or aromatic 5-6 membered ring having 0-3 heteroatoms
selected from O, P, S or N, said fused or spiro ring being optionally substituted; R10 = H,(un)substituted-alkyl, -alkenyl, -alkynyl, -cycloalkyl, -heterocyclyl, -heteroaryl, or aryl; X = (un)substituted-alkylene chain which optionally may have 0-3 heteroatoms selected from O, P, S or N; A = saturated, partially saturated, or aromatic 4-7 monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from O, P, S or N ; m = 0 or 1, n = 0-5] and their pharmaceutically acceptable salts are prepared and disclosed as CCR5 antagonists. Thus, II was prepared by amidation of cis-4-{2-[3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-

yl]ethyl}-4-phenylcyclohexanamine (preparation given) with 3-(aminosulfonyl)-4-chlorobenzoic acid. I have pIC50 values of ≥5 in assays for CCR5 antagonism. As CCR5 antagonists, I are useful for the treatment of viral infections (particularly HIV infection).

IT 714967-95-0P 714967-96-1P 714967-97-2P
714967-98-3P 714967-99-4P 714968-00-0P
714968-02-2P 714968-03-3P 714968-04-4P
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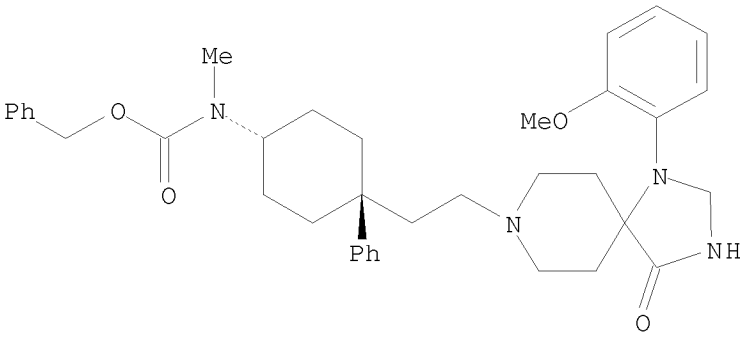
714968-20-4P 714968-21-5P 714968-22-6P
714968-23-7P 714968-24-8P 714968-25-9P
714968-27-1P 714968-28-2P 714968-29-3P
714968-30-6P 716361-32-9P, GSK 259211A
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclylalkyl substituted cyclohexanes derivs. as CCR5 antagonists)

RN 714967-95-0 CAPLUS

CN Carbamic acid, [trans-4-[2-[1-(2-methoxyphenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

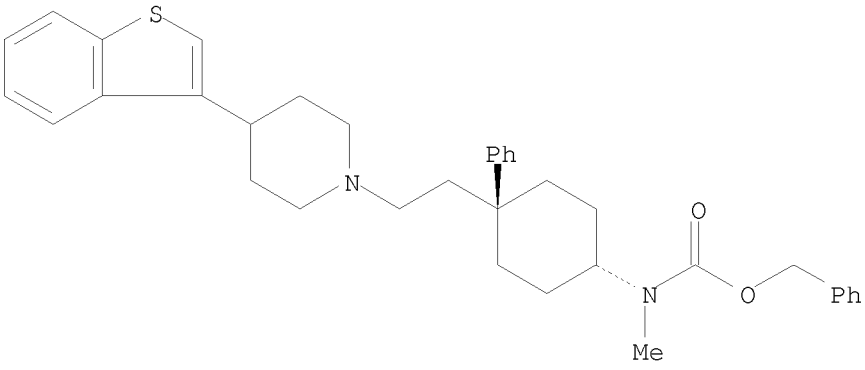
Relative stereochemistry.



RN 714967-96-1 CAPLUS

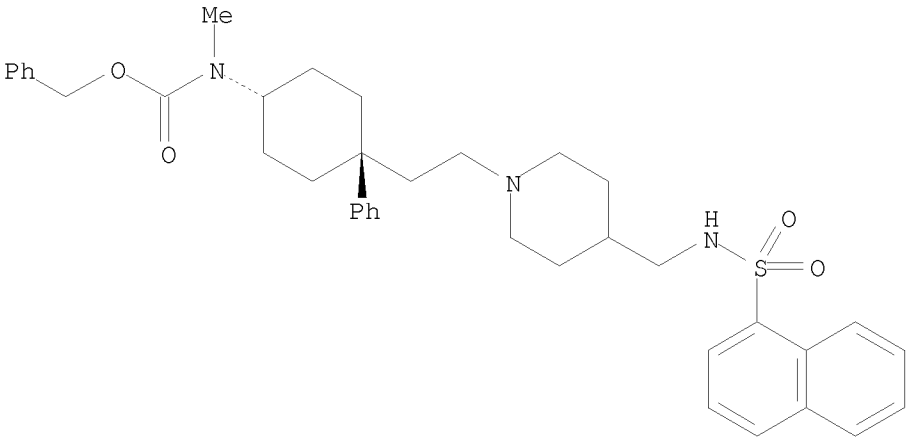
CN Carbamic acid, [trans-4-[2-(4-benzo[b]thien-3-yl-1-piperidinyl)ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



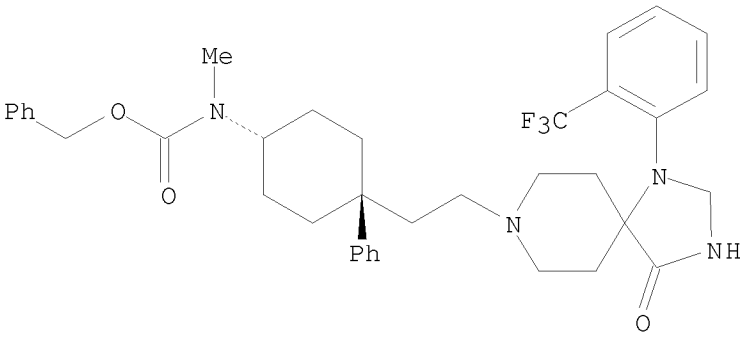
RN 714967-97-2 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylsulfonyl)amino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



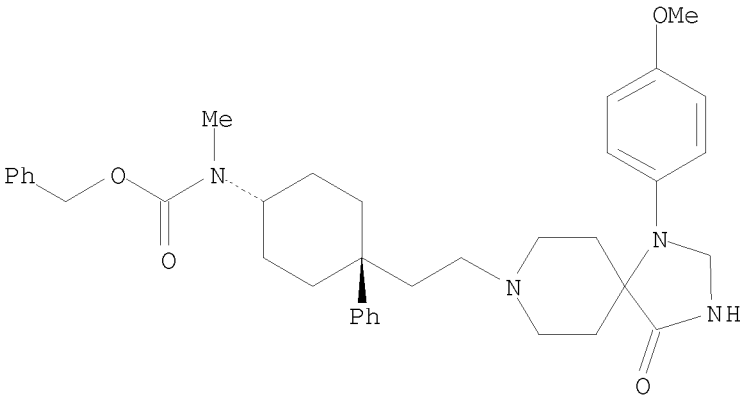
RN 714967-98-3 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-oxo-1-[2-(trifluoromethyl)phenyl]-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



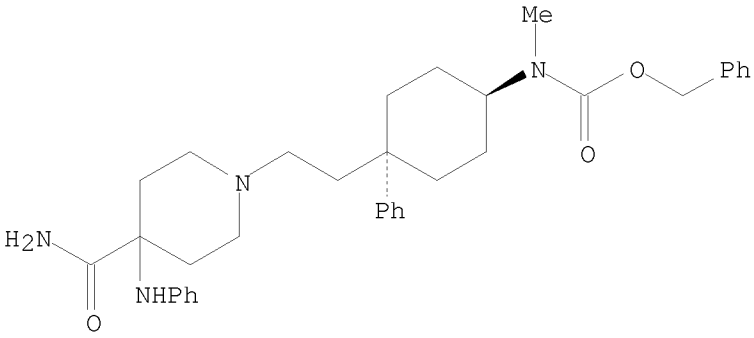
RN 714967-99-4 CAPLUS
CN Carbamic acid, [trans-4-[2-[1-(4-methoxyphenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



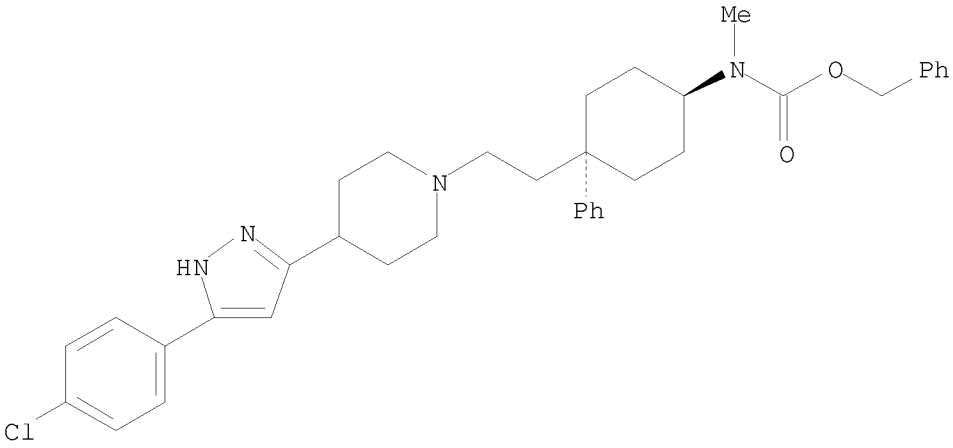
RN 714968-00-0 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-(aminocarbonyl)-4-(phenylamino)-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



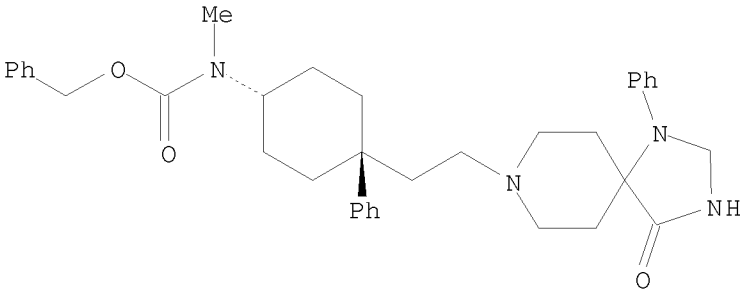
RN 714968-02-2 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[5-(4-chlorophenyl)-1H-pyrazol-3-yl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



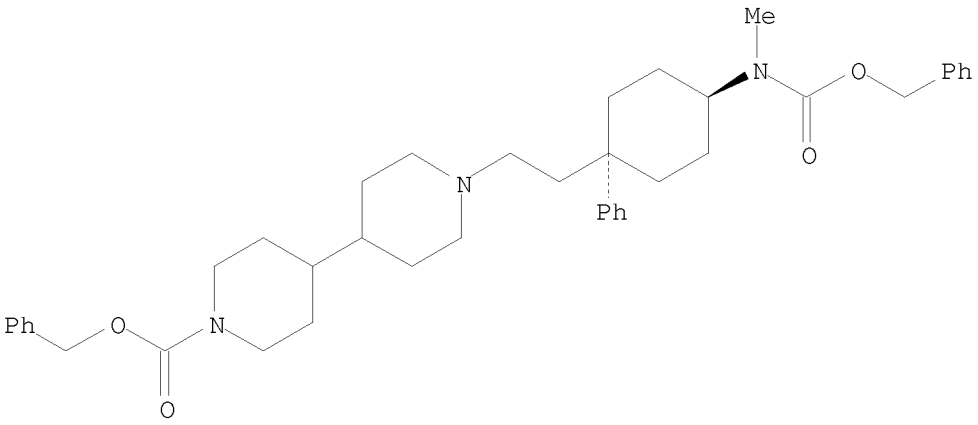
RN 714968-03-3 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



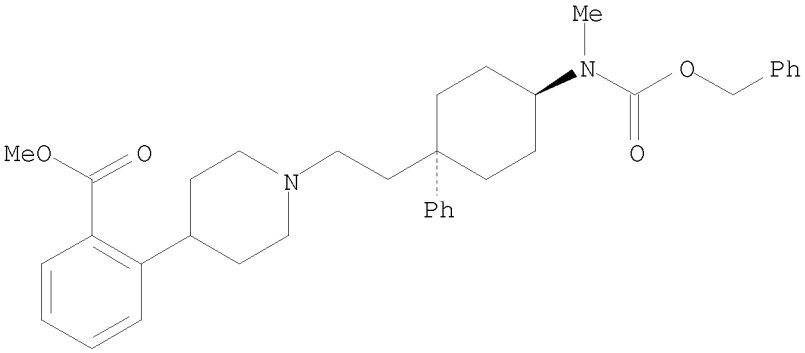
RN 714968-04-4 CAPLUS
CN [4,4'-Bipiperidine]-1-carboxylic acid, 1'-[2-[trans-4-[methyl[(phenylmethoxy)carbonyl]amino]-1-phenylcyclohexyl]ethyl]-, phenylmethyl ester (CA INDEX NAME)

Relative stereochemistry.



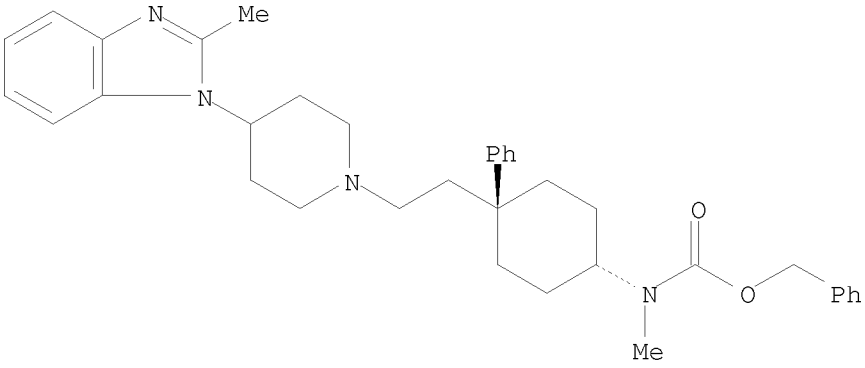
RN 714968-05-5 CAPLUS
CN Benzoic acid, 2-[1-[2-[trans-4-[methyl[(phenylmethoxy)carbonyl]amino]-1-phenylcyclohexyl]ethyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)

Relative stereochemistry.



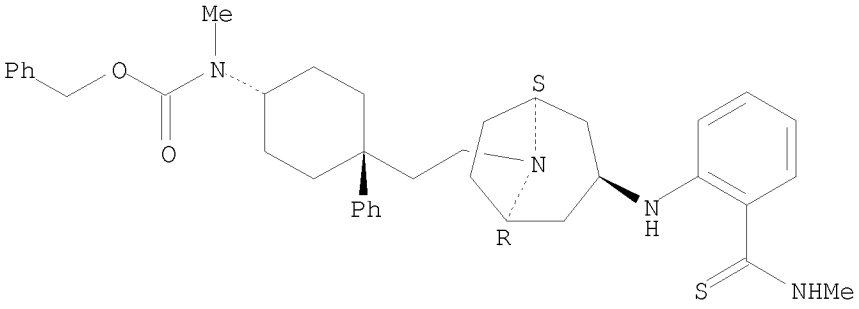
RN 714968-06-6 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-(2-methyl-1H-benzimidazol-1-yl)-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



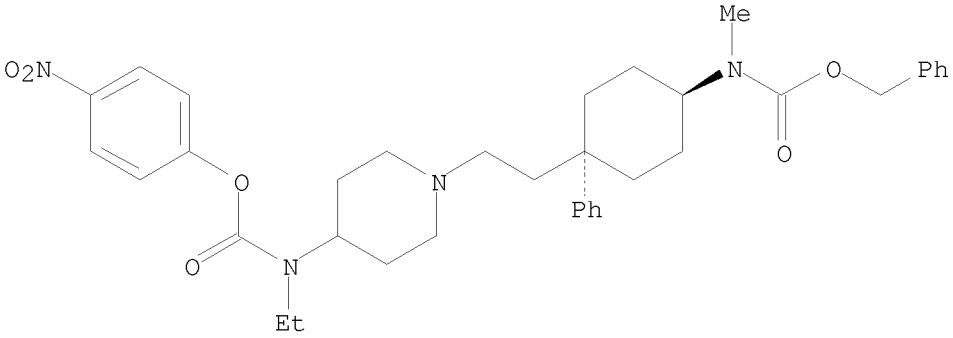
RN 714968-07-7 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[(3-endo)-3-[[2-[(methylamino)thioxomethyl]phenyl]amino]-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



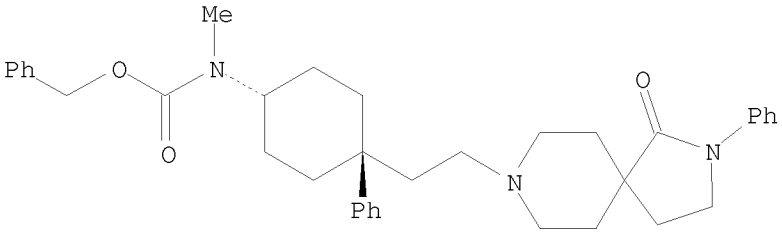
RN 714968-08-8 CAPLUS
CN Carbamic acid, ethyl[1-[2-[trans-4-[methyl[(phenylmethoxy)carbonyl]amino]-1-phenylcyclohexyl]ethyl]-4-piperidinyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 714968-09-9 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-(1-oxo-2-phenyl-2,8-diazaspiro[4.5]dec-8-yl)ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

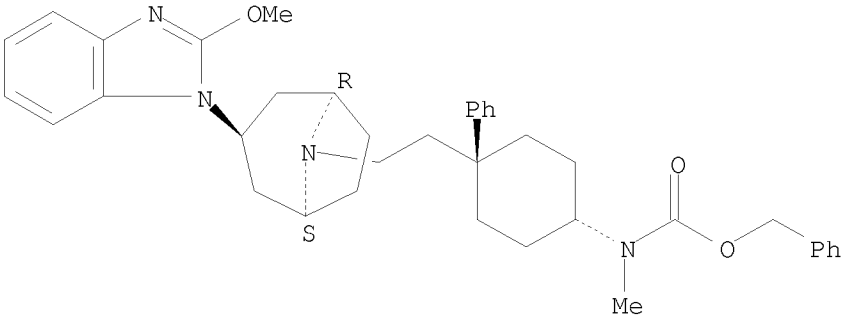
Relative stereochemistry.



RN 714968-10-2 CAPLUS
CN Carbamic acid, [trans-4-[2-[(3-endo)-3-(2-methoxy-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl

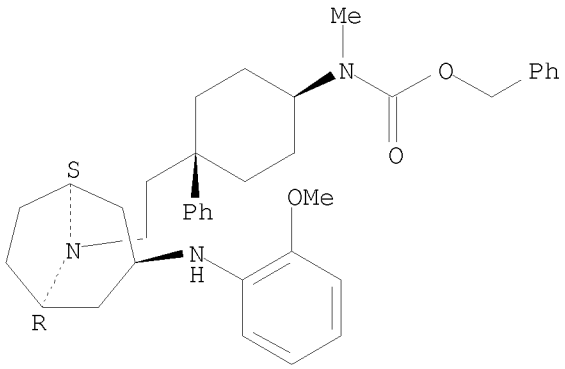
ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



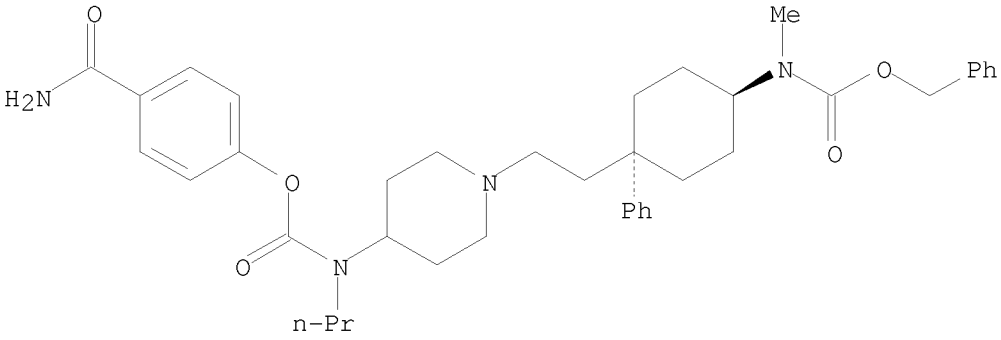
RN 714968-11-3 CAPLUS
CN Carbamic acid, [cis-4-[2-[(3-endo)-3-[(2-methoxyphenyl)amino]-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



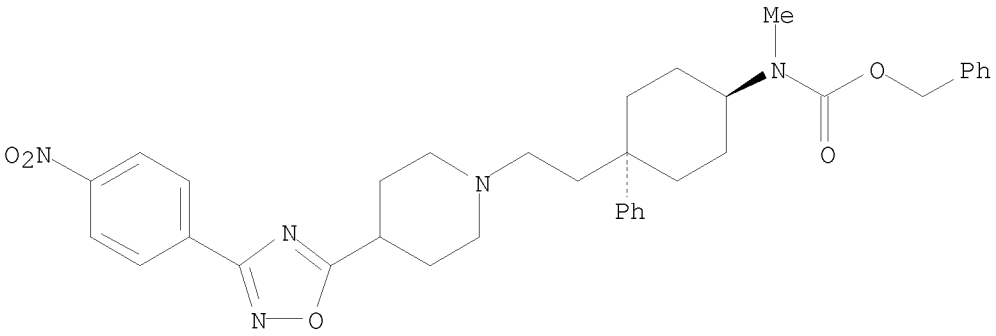
RN 714968-12-4 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[[[4-(aminocarbonyl)phenoxy]carbonyl]propylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



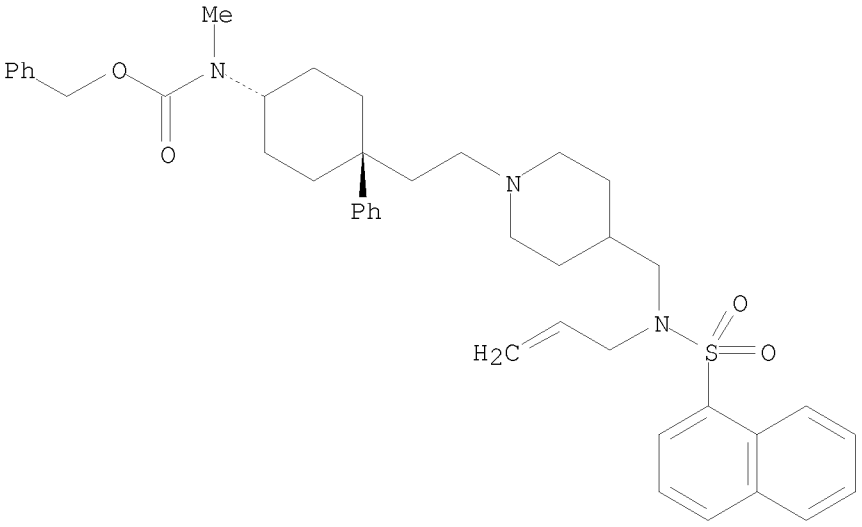
RN 714968-13-5 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



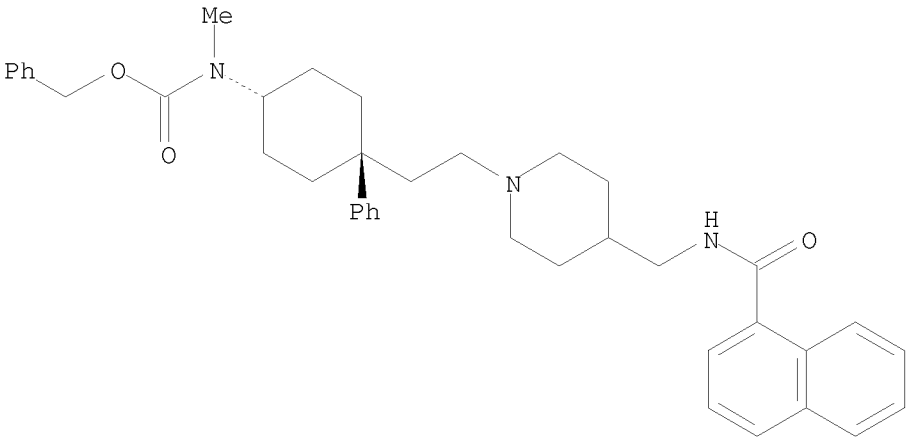
RN 714968-14-6 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylsulfonyl)-2-propenylamino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



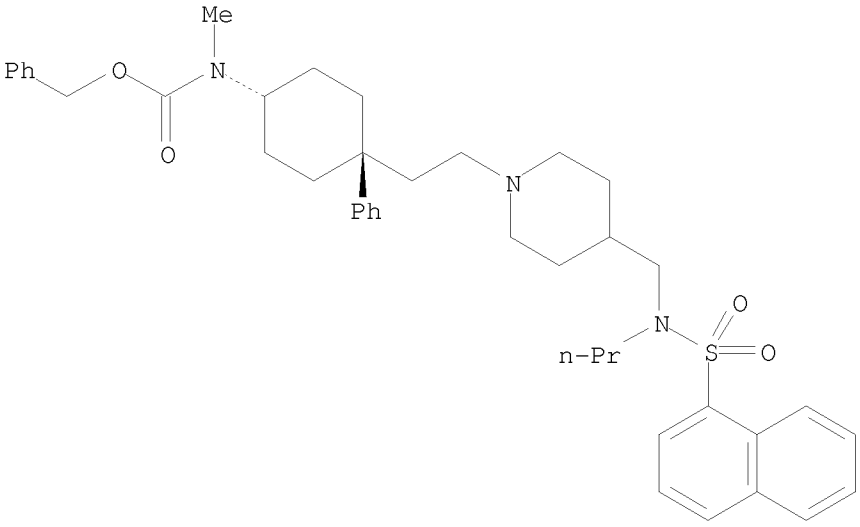
RN 714968-15-7 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylcarbonyl)amino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



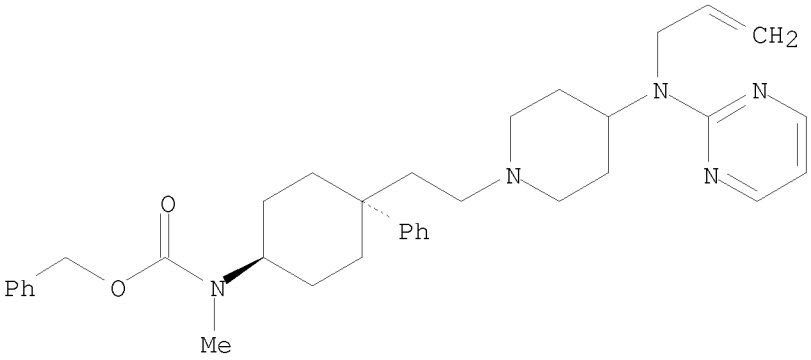
RN 714968-16-8 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylsulfonyl)propylamino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



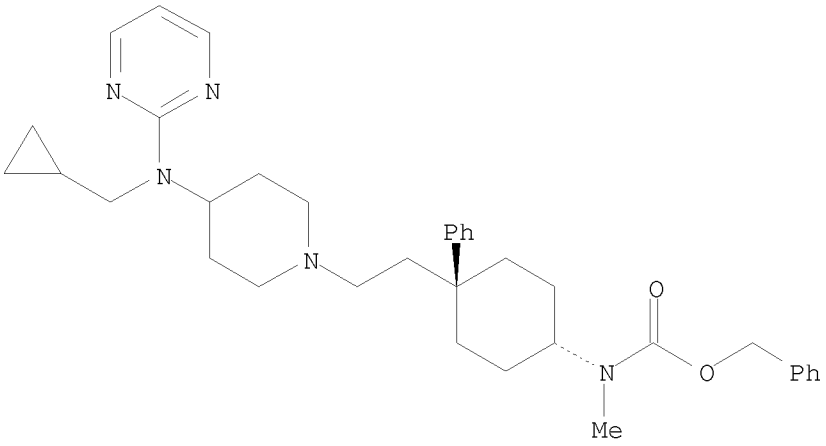
RN 714968-17-9 CAPLUS
CN Carbamic acid, methyl[trans-4-phenyl-4-[2-[4-(2-propenyl-2-pyrimidinylamino)-1-piperidinyl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



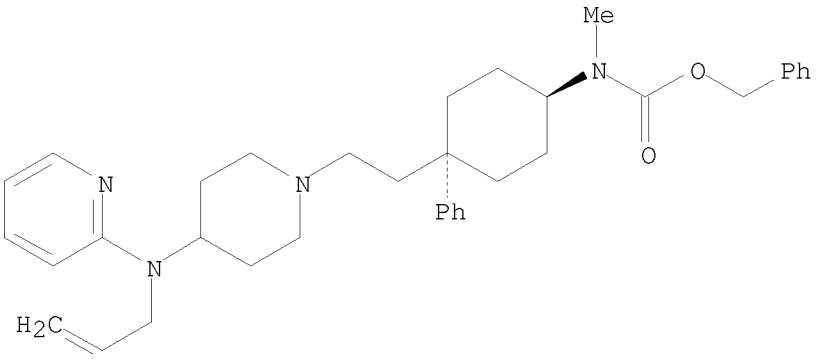
RN 714968-18-0 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(cyclopropylmethyl)-2-pyrimidinylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



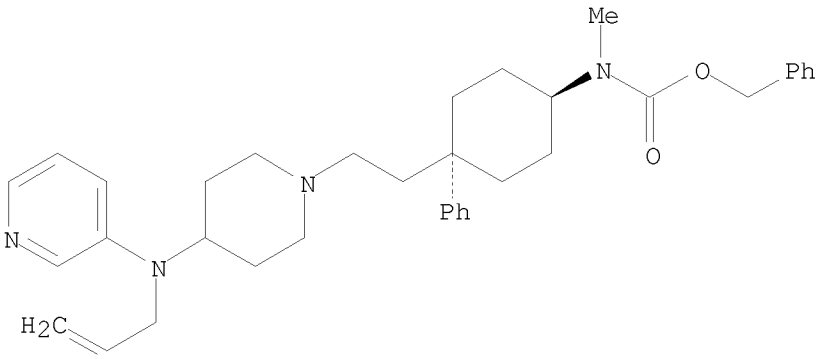
RN 714968-19-1 CAPLUS
CN Carbamic acid, methyl[trans-4-phenyl-4-[2-[4-(2-propenyl-2-pyridinylamino)-1-piperidinyl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



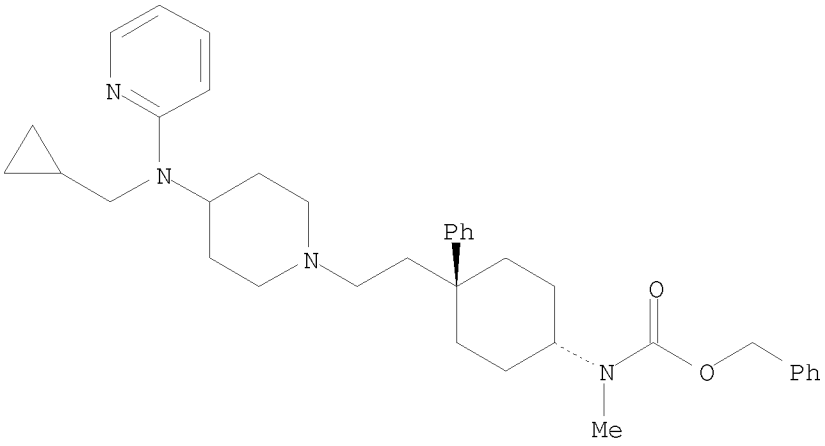
RN 714968-20-4 CAPLUS
CN Carbamic acid, methyl[trans-4-phenyl-4-[2-[4-(2-propenyl-3-pyridinylamino)-1-piperidinyl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



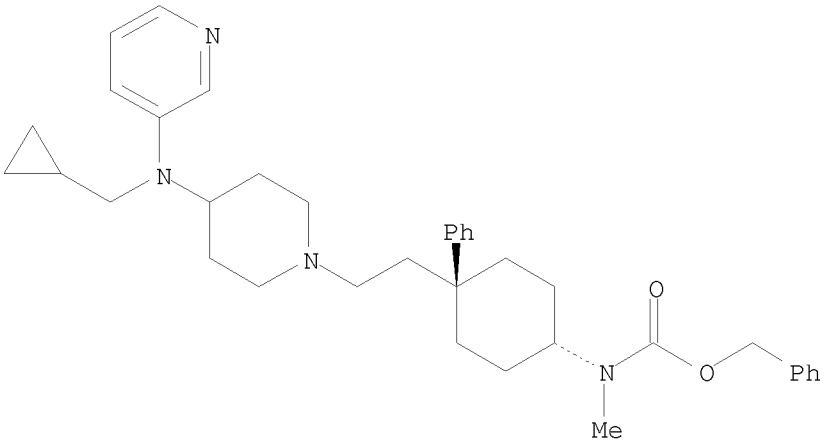
RN 714968-21-5 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(cyclopropylmethyl)-2-pyridinylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



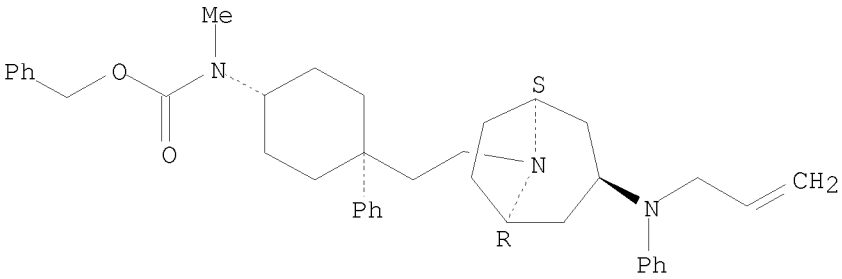
RN 714968-22-6 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(cyclopropylmethyl)-3-pyridinylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



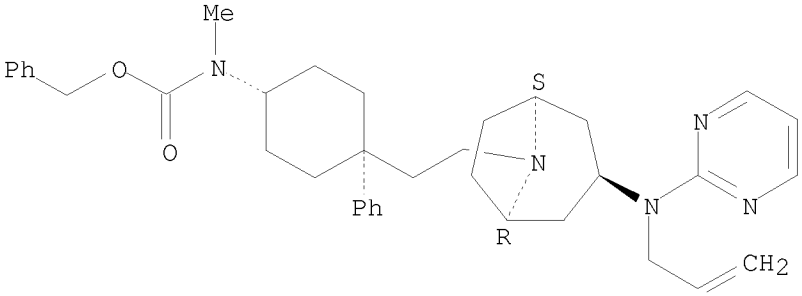
RN 714968-23-7 CAPLUS
CN Carbamic acid, methyl[cis-4-phenyl-4-[2-[(3-endo)-3-(phenyl-2-propenylamino)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



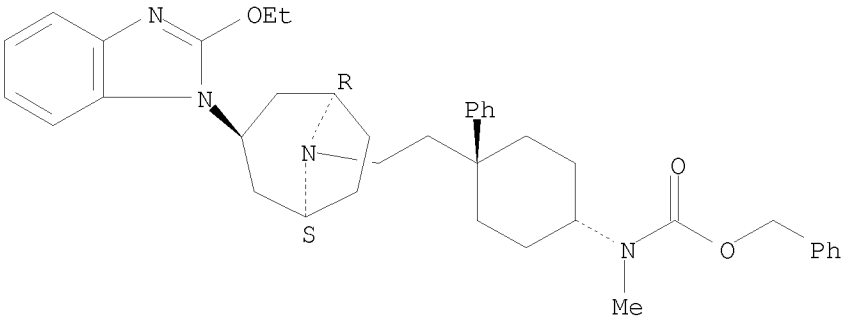
RN 714968-24-8 CAPLUS
CN Carbamic acid, methyl[cis-4-phenyl-4-[2-[(3-endo)-3-(2-propenyl-2-pyrimidinylamino)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



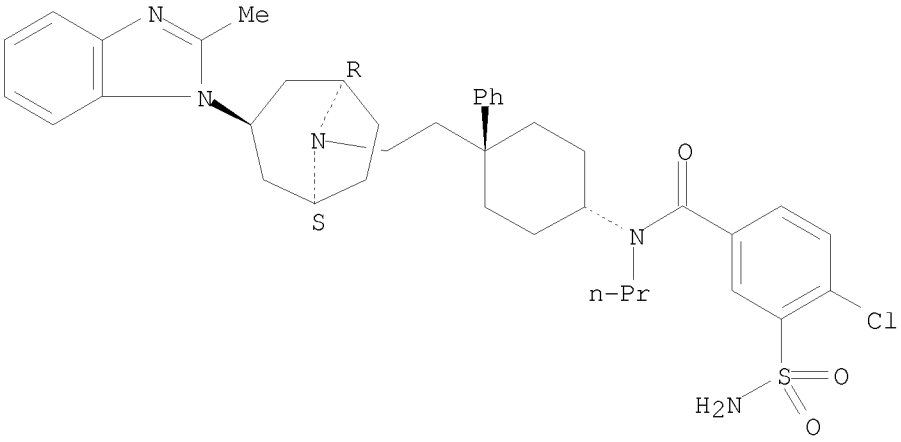
RN 714968-25-9 CAPLUS
CN Carbamic acid, [trans-4-[2-[(3-endo)-3-(2-ethoxy-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



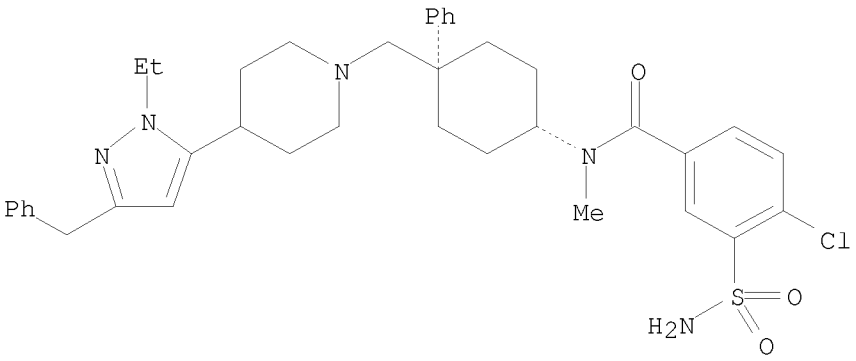
RN 714968-27-1 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-N-propyl- (CA INDEX NAME)

Relative stereochemistry.



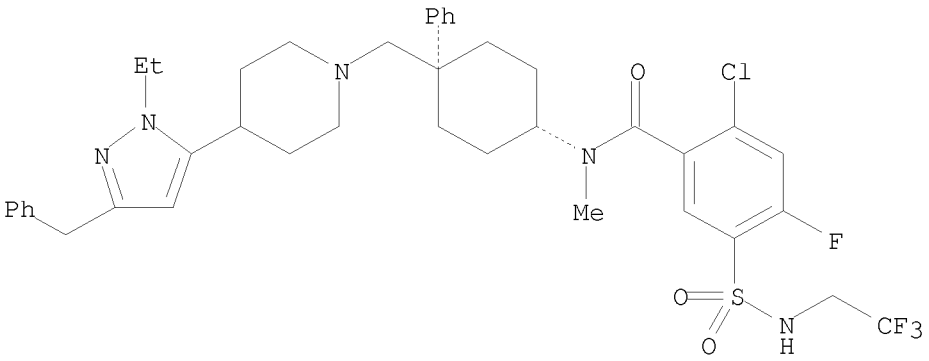
RN 714968-28-2 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[trans-4-[[4-[1-ethyl-3-(phenylmethyl)-1H-pyrazol-5-yl]-1-piperidinyl]methyl]-4-phenylcyclohexyl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.



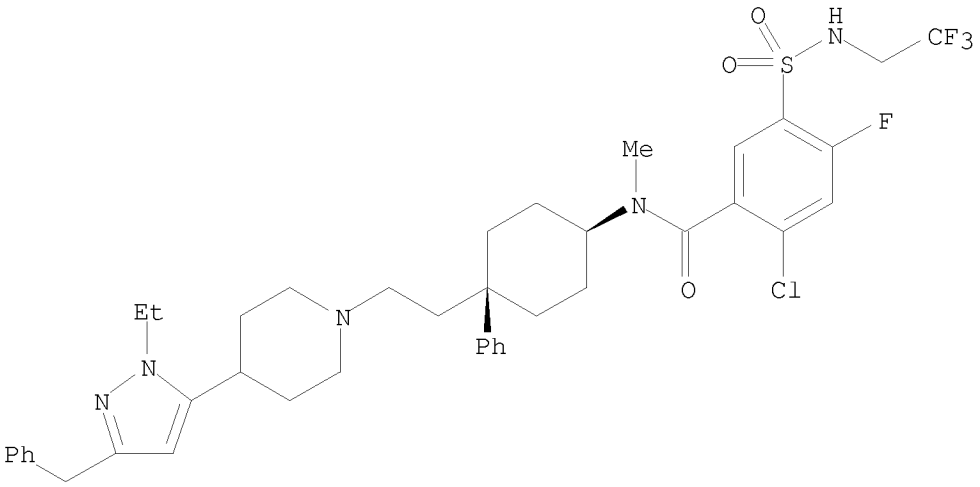
RN 714968-29-3 CAPLUS
CN Benzamide, 2-chloro-N-[trans-4-[[4-[1-ethyl-3-(phenylmethyl)-1H-pyrazol-5-yl]-1-piperidinyl]methyl]-4-phenylcyclohexyl]-4-fluoro-N-methyl-5-[[(2,2,2-trifluoroethyl)amino]sulfonyl]- (CA INDEX NAME)

Relative stereochemistry.



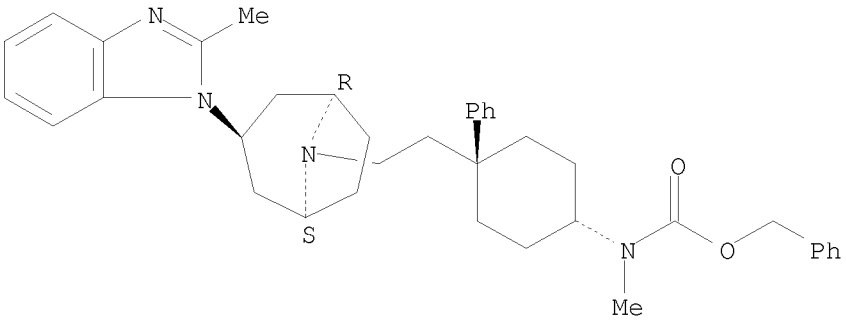
RN 714968-30-6 CAPLUS
CN Benzamide, 2-chloro-N-[cis-4-[2-[4-[1-ethyl-3-(phenylmethyl)-1H-pyrazol-5-yl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-4-fluoro-N-methyl-5-[[(2,2,2-trifluoroethyl)amino]sulfonyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 716361-32-9 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

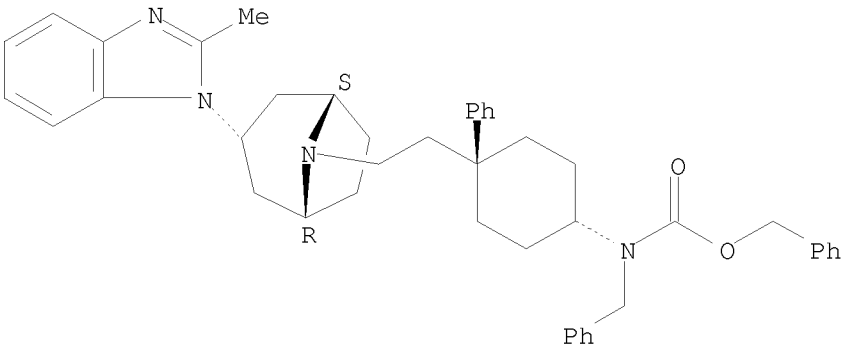
Relative stereochemistry.



IT 714967-84-7P 714968-33-9P 714968-40-8P
716343-88-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclylalkyl substituted cyclohexanes derivs. as CCR5 antagonists)

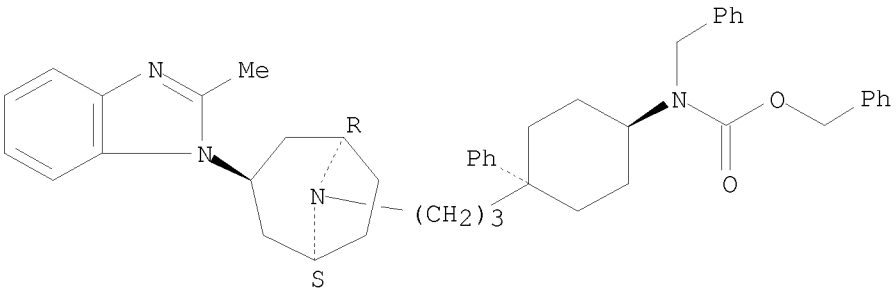
RN 714967-84-7 CAPLUS
CN Carbamic acid, [trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

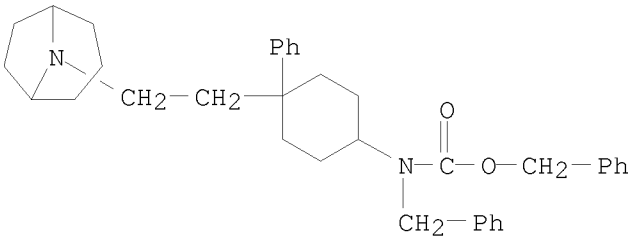


RN 714968-33-9 CAPLUS
CN Carbamic acid, [trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

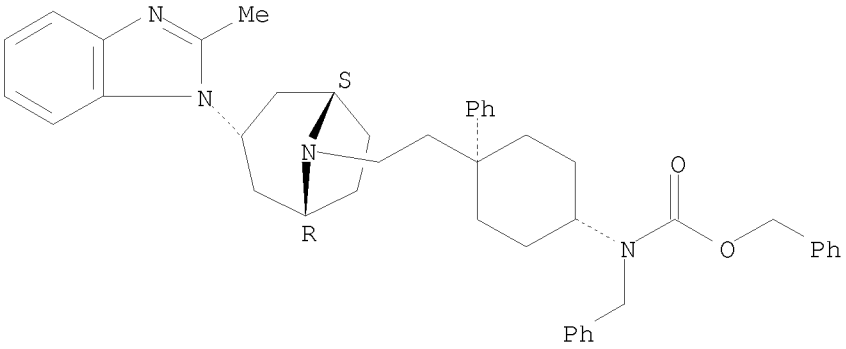


RN 714968-40-8 CAPLUS
CN Carbamic acid, [4-[2-(8-azabicyclo[3.2.1]oct-8-yl)ethyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 716343-88-3 CAPLUS
CN Carbamic acid, [cis-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.85	186.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.80	-0.80

FILE 'REGISTRY' ENTERED AT 10:29:26 ON 22 OCT 2008

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 OCT 2008 HIGHEST RN 1064205-90-8
DICTIONARY FILE UPDATES: 21 OCT 2008 HIGHEST RN 1064205-90-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

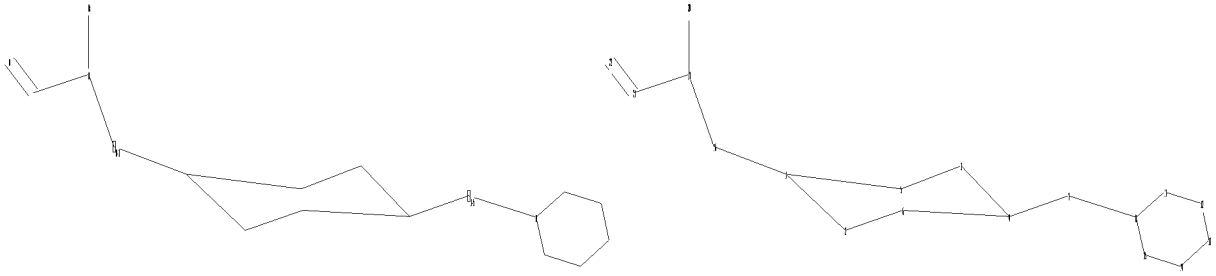
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10-538,135-1a.str



```
chain nodes :
7  16  17  20  21  22
ring nodes :
1  2  3  4  5  6  8  11  12  13  14  15
chain bonds :
1-16  4-7  7-8  16-17  17-20  17-21  21-22
ring bonds :
1-2  1-5  2-6  3-4  3-5  4-6  8-11  8-15  11-12  12-13  13-14  14-15
exact/norm bonds :
1-2  1-5  2-6  3-4  3-5  4-6  7-8  8-11  8-15  11-12  12-13  13-14  14-15  16-17
17-20  17-21  21-22
exact bonds :
1-16  4-7


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:Atom  11:Atom  12:Atom
13:Atom  14:Atom  15:Atom  16:CLASS  17:CLASS  20:CLASS  21:CLASS  22:CLASS




L5      STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5              STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

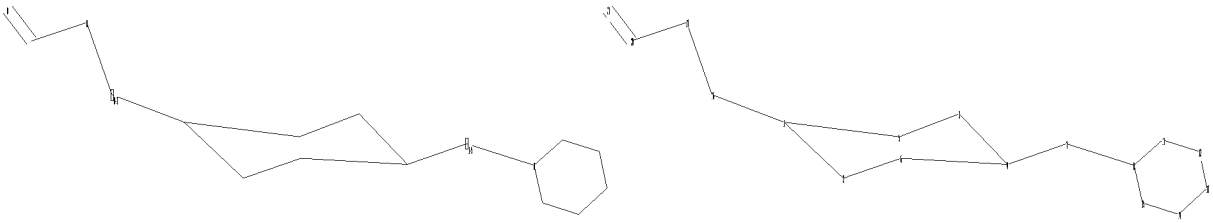

=> s l5 sss sam
SAMPLE SEARCH INITIATED 10:29:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    23664 TO ITERATE

  8.5% PROCESSED     2000 ITERATIONS                                2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       464072 TO   482488
PROJECTED ANSWERS:             182 TO      764

L6            2 SEA SSS SAM L5

=>
Uploading C:\Program Files\Stnexp\Queries\10-538,135-1b.str
```



chain nodes :
7 16 17 20 21
ring nodes :
1 2 3 4 5 6 8 11 12 13 14 15
chain bonds :
1-16 4-7 7-8 16-17 17-20 20-21
ring bonds :
1-2 1-5 2-6 3-4 3-5 4-6 8-11 8-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-2 1-5 2-6 3-4 3-5 4-6 7-8 8-11 8-15 11-12 12-13 13-14 14-15 16-17
17-20 20-21
exact bonds :
1-16 4-7

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 20:CLASS 21:CLASS

L7 STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l7 sss sam
SAMPLE SEARCH INITIATED 10:32:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23664 TO ITERATE

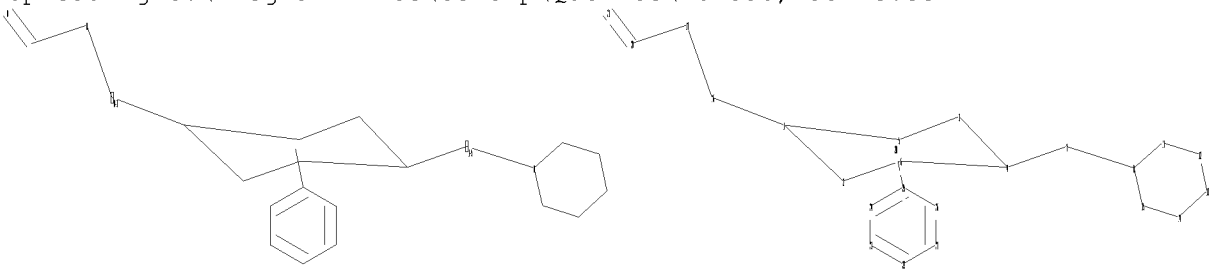
8.5% PROCESSED 2000 ITERATIONS 37 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 464072 TO 482488
PROJECTED ANSWERS: 7500 TO 10010

L8 37 SEA SSS SAM L7

=>
Uploading C:\Program Files\Stnexp\Queries\10-538,135-1c.str



chain nodes :
7 16 17 20 21
ring nodes :
1 2 3 4 5 6 8 11 12 13 14 15 22 23 24 25 26 27
chain bonds :
1-16 4-7 7-8 16-17 17-20 20-21
ring bonds :
1-2 1-5 2-6 3-4 3-5 4-6 8-11 8-15 11-12 12-13 13-14 14-15 22-23 22-27
23-24 24-25 25-26 26-27
exact/norm bonds :
1-2 1-5 2-6 3-4 3-5 4-6 7-8 8-11 8-15 11-12 12-13 13-14 14-15 16-17
17-20 20-21
exact bonds :
1-16 4-7
normalized bonds :
22-23 22-27 23-24 24-25 25-26 26-27

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom
24:Atom 25:Atom

26:Atom 27:Atom 28:Atom

L9 STRUCTURE UPLOADED

=> d l9
L9 HAS NO ANSWERS
L9 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

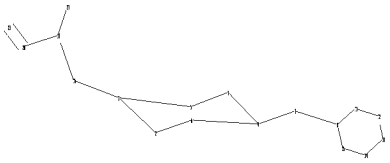
=> s l9 sss sam
SAMPLE SEARCH INITIATED 10:33:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 22960 TO ITERATE

8.7% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 450130 TO 468270
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=>
Uploading C:\Program Files\Stnexp\Queries\10-538,135-d.str



chain nodes :
7 16 17 20 21 23
ring nodes :
1 2 3 4 5 6 8 11 12 13 14 15
chain bonds :
1-16 4-7 7-8 16-17 17-20 17-23 20-21
ring bonds :
1-2 1-5 2-6 3-4 3-5 4-6 8-11 8-15 11-12 12-13 13-14 14-15
exact/norm bonds :
1-2 1-5 2-6 3-4 3-5 4-6 7-8 8-11 8-15 11-12 12-13 13-14 14-15 16-17
17-20 17-23 20-21
exact bonds :
1-16 4-7

G1:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 20:CLASS 21:CLASS 23:CLASS

L11 STRUCTURE UPLOADED

=> d l11

```
L11 HAS NO ANSWERS
L11             STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

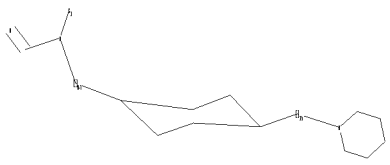

=> s l11 sss sam
SAMPLE SEARCH INITIATED 10:36:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    23664 TO ITERATE

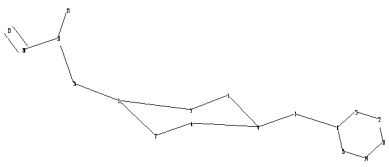
  8.5% PROCESSED     2000 ITERATIONS                                37 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       464072 TO   482488
PROJECTED ANSWERS:            7500 TO    10010

L12          37 SEA SSS SAM L11

=>
Uploading C:\Program Files\Stnexp\Queries\10-538,135-1e.str
```





```
chain nodes :
7  16  17  20  21  23
```

```
ring nodes :
1  2  3  4  5  6  8  11  12  13  14  15
chain bonds :
1-16  4-7  7-8  16-17  17-20  17-23  20-21
ring bonds :
1-2  1-5  2-6  3-4  3-5  4-6  8-11  8-15  11-12  12-13  13-14  14-15
exact/norm bonds :
7-8  8-11  8-15  11-12  12-13  13-14  14-15  16-17  17-20  17-23  20-21
exact bonds :
1-2  1-5  1-16  2-6  3-4  3-5  4-6  4-7
isolated ring systems :
containing 1 :


G1:H,Ak

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:Atom  11:Atom  12:Atom
13:Atom  14:Atom  15:Atom  16:CLASS  17:CLASS  20:CLASS  21:CLASS  23:CLASS




L13     STRUCTURE UPLOADED

=> d l13
L13 HAS NO ANSWERS
L13             STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l13 sss sam
SAMPLE SEARCH INITIATED 10:38:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     4187 TO ITERATE

 47.8% PROCESSED     2000 ITERATIONS                                 18 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        79860 TO    87620
PROJECTED ANSWERS:             385 TO     1121

L14          18 SEA SSS SAM L13

=> s l13 sss full
FULL SEARCH INITIATED 10:38:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    84507 TO ITERATE

100.0% PROCESSED    84507 ITERATIONS                               956 ANSWERS
SEARCH TIME: 00.00.02
```

```
L15         956 SEA SSS FUL L13

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     185.26     372.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -0.80

FILE 'CAPLUS' ENTERED AT 10:38:53 ON 22 OCT 2008
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FILE COVERS 1907 - 22 Oct 2008  VOL 149 ISS 17
FILE LAST UPDATED: 21 Oct 2008  (20081021/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

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L16           1 L3

=> s l15
L17          98 L15

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L18          38 L15 AND (PY<2003 OR AY<2003 OR PRY<2003)

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YOU HAVE REQUESTED DATA FROM 38 ANSWERS - CONTINUE? Y/(N):y

L18  ANSWER 1 OF 38  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:        2004:531360  CAPLUS <<LOGINID::20081022>>
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DOCUMENT NUMBER: 141:88873
TITLE: Preparation of heterocyclylalkyl substituted cyclohexyl compounds as CCR5 antagonists
INVENTOR(S): Duan, Maosheng; Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054581	A2	20040701	WO 2003-US39732	20031212 <--
WO 2004054581	A3	20050203		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003297048	A1	20040709	AU 2003-297048	20031212 <--
EP 1569647	A2	20050907	EP 2003-813435	20031212 <--
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
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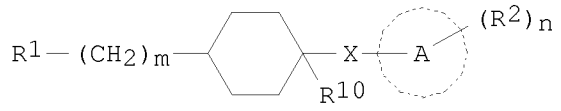
AT 405269	T	20080915	AT 2003-813435	20031212 <--
US 20060122166	A1	20060608	US 2005-538135	20050609 <--
PRIORITY APPLN. INFO.:			US 2002-433552P P	20021213 <--
			WO 2003-US39732 W	20031212

OTHER SOURCE(S): MARPAT 141:88873
GI



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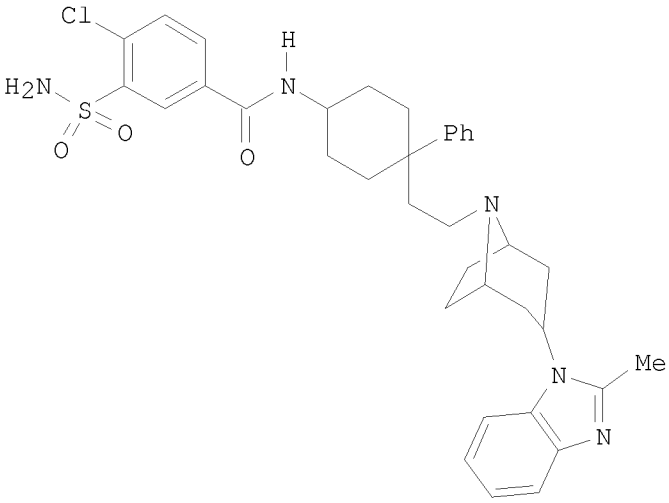

II

AB Title compds. I [R1 = (un)substituted saturated, partially saturated, or aromatic 4-7 monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from O, P, S or N, optionally attached through alkylene chain, substituted-amine, -amide, etc.; R2 = OH, halogen (un)substituted-alkyl, -alkoxy, -aryl, -heteroaryl, -cycloalkyl, etc., optionally two adjacent R2s taken together form a fused, saturated, partially saturated or aromatic 5-6 membered ring having 0-3 heteroatoms selected from O, P, S, or N, or two geminal R2s optionally taken together from a spiro, saturated, partially saturated or aromatic 5-6 membered ring having 0-3 heteroatoms selected from O, P, S or N, said fused or spiro ring being optionally substituted; R10 = H,(un)substituted-alkyl, -alkenyl, -alkynyl, -cycloalkyl, -heterocyclyl, -heteroaryl, or aryl; X = (un)substituted-alkylene chain which optionally may have 0-3 heteroatoms selected from O, P, S or N; A = saturated, partially saturated, or aromatic 4-7 monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from O, P, S or N ; m = 0 or 1, n = 0-5] and their pharmaceutically acceptable salts are prepared and disclosed as CCR5 antagonists. Thus, II was prepared by amidation of cis-4-{2-[3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl}-4-phenylcyclohexanamine (preparation given) with 3-(aminosulfonyl)-4-chlorobenzoic acid. I have pIC50 values of ≥5 in assays for CCR5 antagonism. As CCR5 antagonists, I are useful for the treatment of viral infections (particularly HIV infection).

IT 714967-86-9P 714967-87-0P 714967-88-1P
714967-89-2P 714967-90-5P 714967-91-6P
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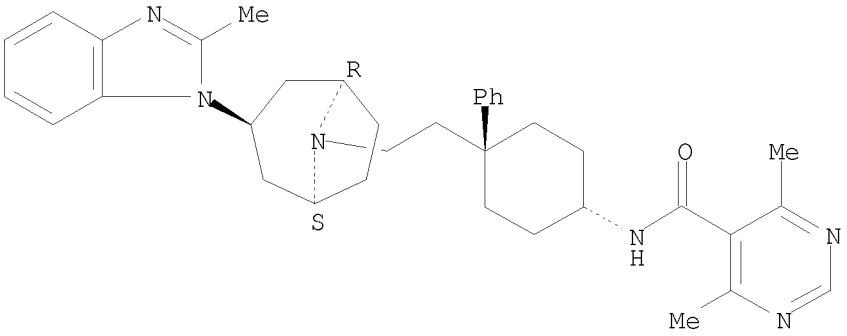
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclylalkyl substituted cyclohexanes derivs. as CCR5 antagonists)

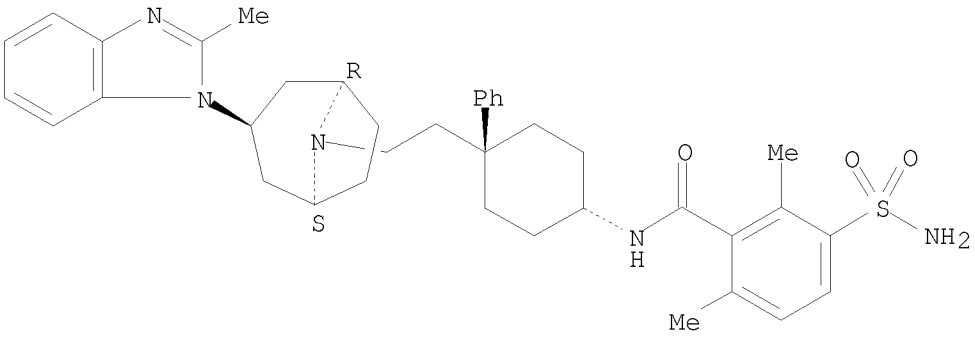
RN 714967-86-9 CAPLUS
CN 5-Pyrimidinecarboxamide, 4,6-dimethyl-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



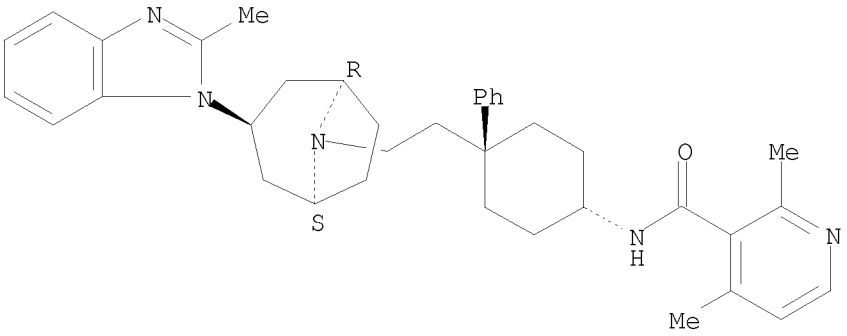
RN 714967-87-0 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-2,6-dimethyl-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



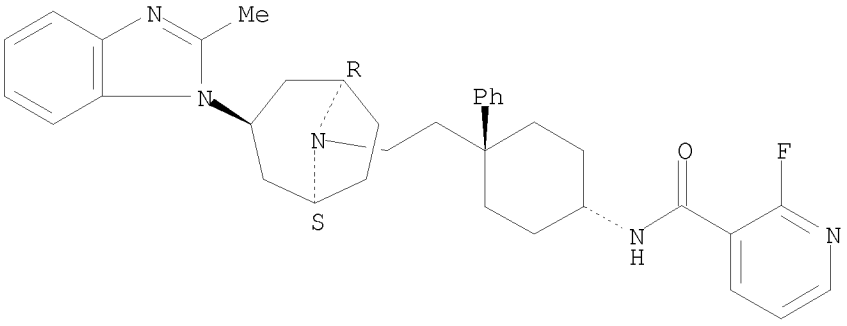
RN 714967-88-1 CAPLUS
CN 3-Pyridinecarboxamide, 2,4-dimethyl-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



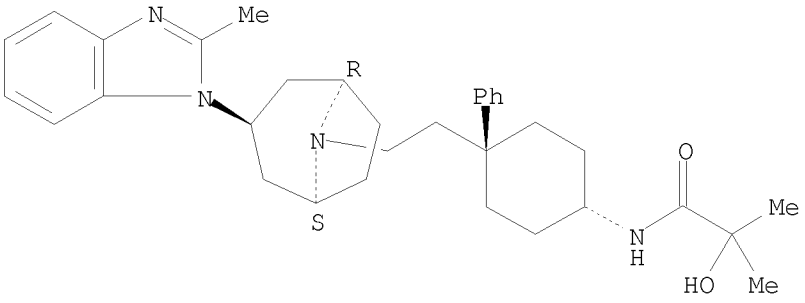
RN 714967-89-2 CAPLUS
CN 3-Pyridinecarboxamide, 2-fluoro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



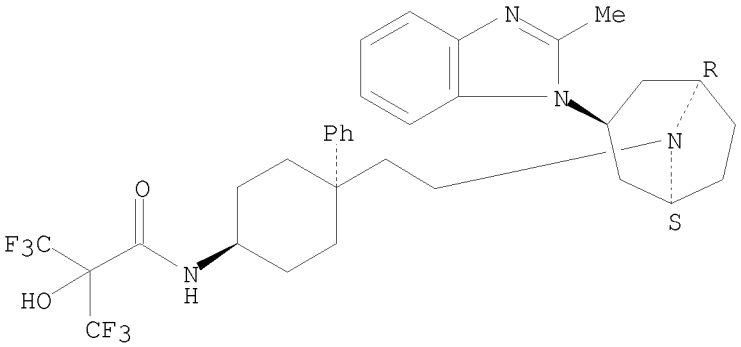
RN 714967-90-5 CAPLUS
CN Propanamide, 2-hydroxy-2-methyl-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



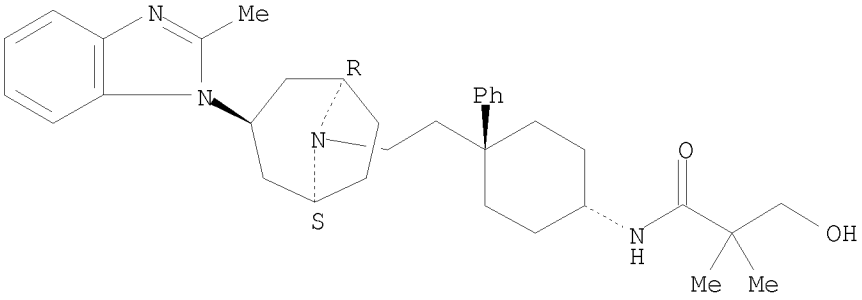
RN 714967-91-6 CAPLUS
CN Propanamide, 3,3,3-trifluoro-2-hydroxy-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-2-(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



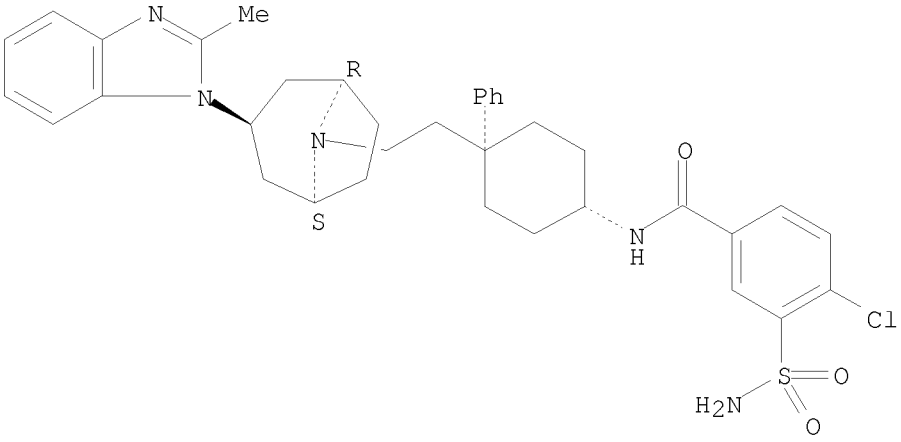
RN 714967-92-7 CAPLUS
CN Propanamide, 3-hydroxy-2,2-dimethyl-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



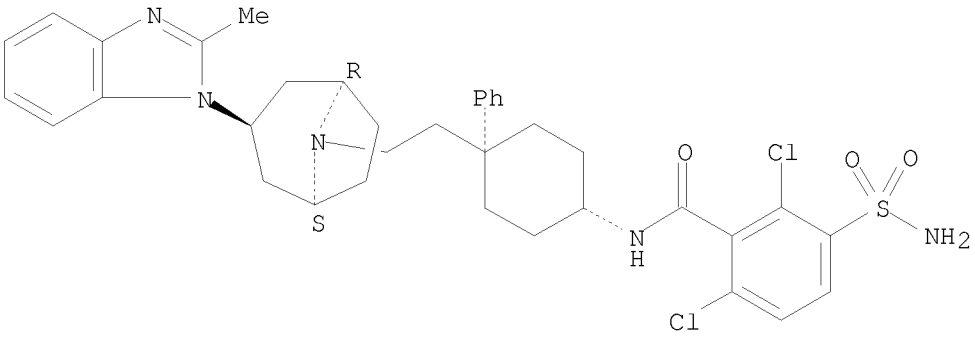
RN 714967-93-8 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[cis-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



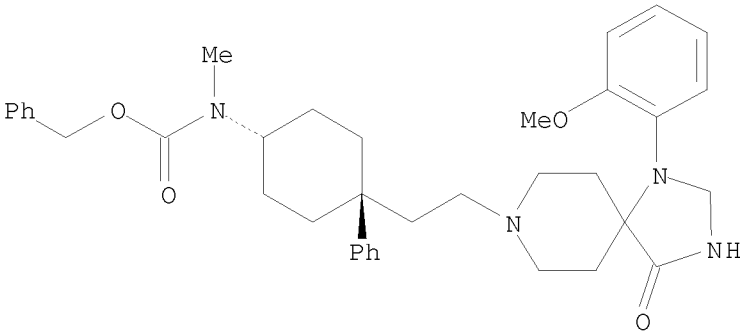
RN 714967-94-9 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-2,6-dichloro-N-[cis-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



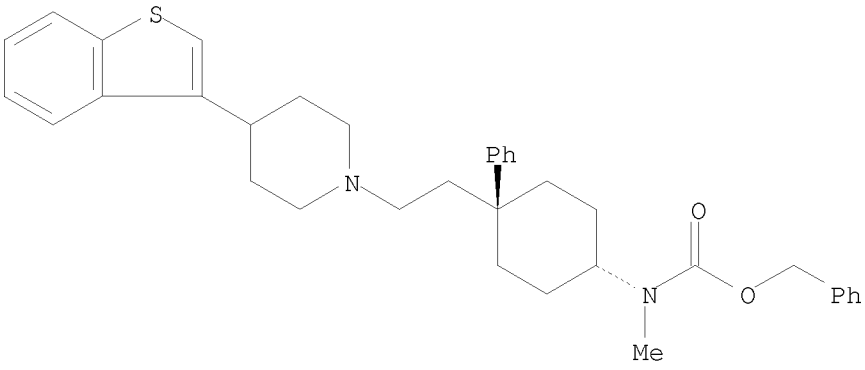
RN 714967-95-0 CAPLUS
CN Carbamic acid, [trans-4-[2-[1-(2-methoxyphenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



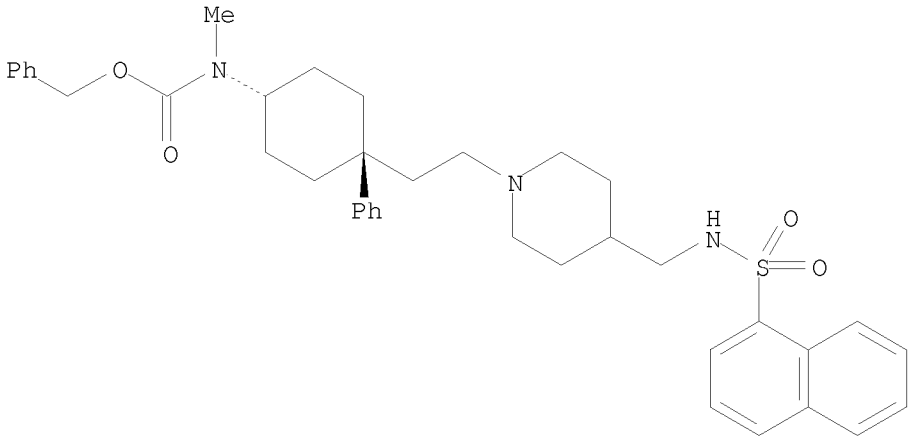
RN 714967-96-1 CAPLUS
CN Carbamic acid, [trans-4-[2-(4-benzo[b]thien-3-yl-1-piperidinyl)ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



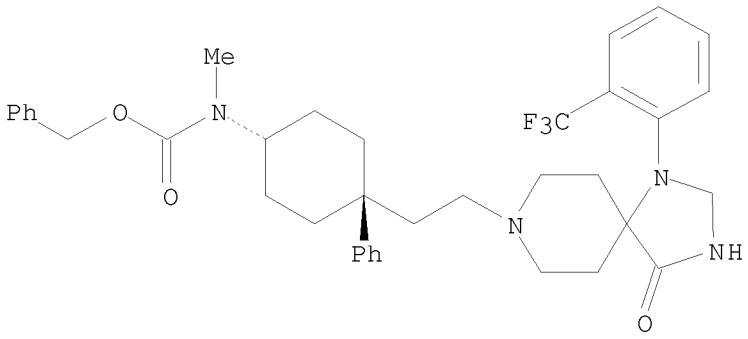
RN 714967-97-2 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylsulfonyl)amino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



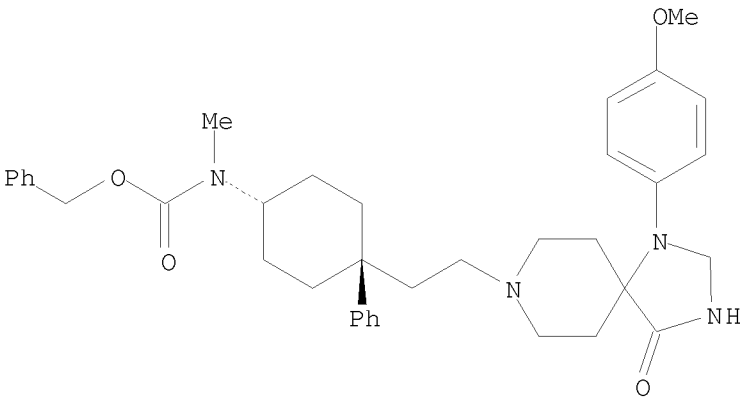
RN 714967-98-3 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-oxo-1-[2-(trifluoromethyl)phenyl]-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



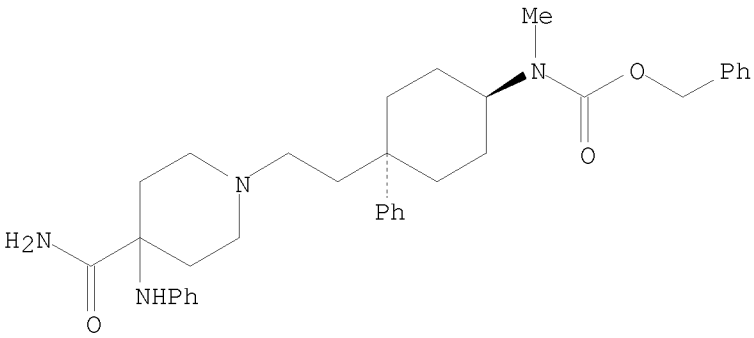
RN 714967-99-4 CAPLUS
CN Carbamic acid, [trans-4-[2-[1-(4-methoxyphenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



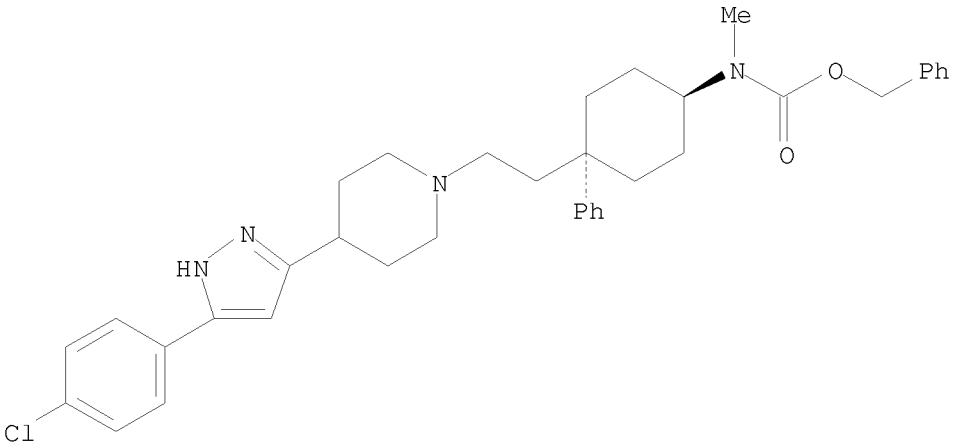
RN 714968-00-0 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-(aminocarbonyl)-4-(phenylamino)-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



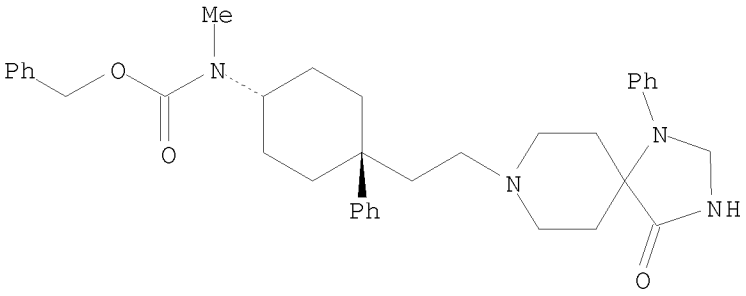
RN 714968-02-2 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[5-(4-chlorophenyl)-1H-pyrazol-3-yl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



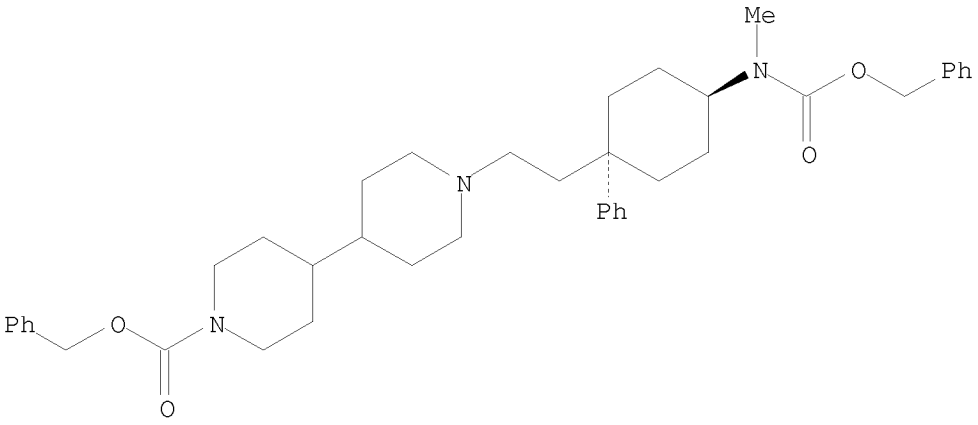
RN 714968-03-3 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



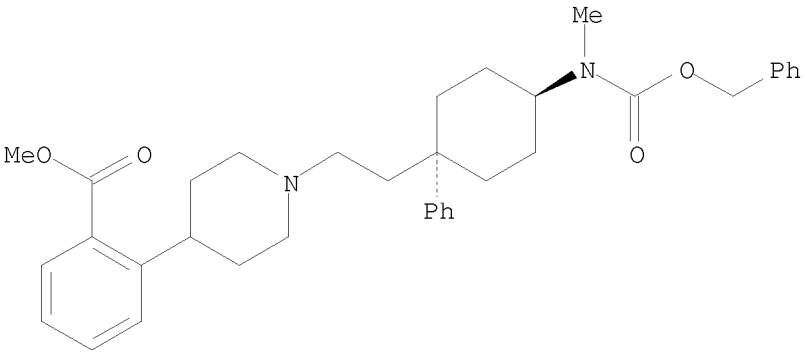
RN 714968-04-4 CAPLUS
CN [4,4'-Bipiperidine]-1-carboxylic acid, 1'-[2-[trans-4-[methyl[(phenylmethoxy)carbonyl]amino]-1-phenylcyclohexyl]ethyl]-, phenylmethyl ester (CA INDEX NAME)

Relative stereochemistry.



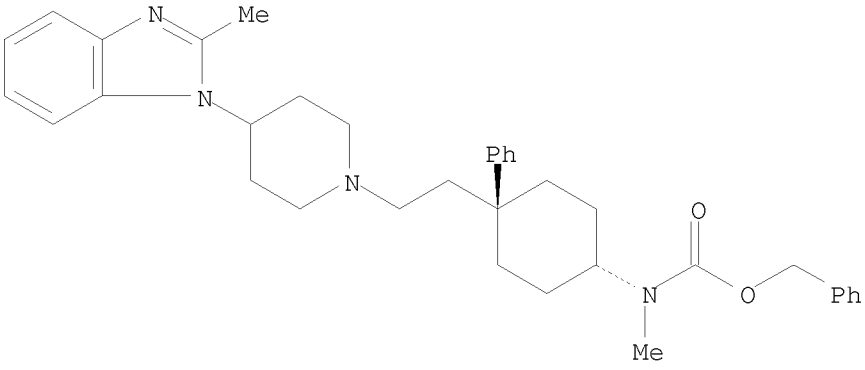
RN 714968-05-5 CAPLUS
CN Benzoic acid, 2-[1-[2-[trans-4-[methyl[(phenylmethoxy)carbonyl]amino]-1-phenylcyclohexyl]ethyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)

Relative stereochemistry.



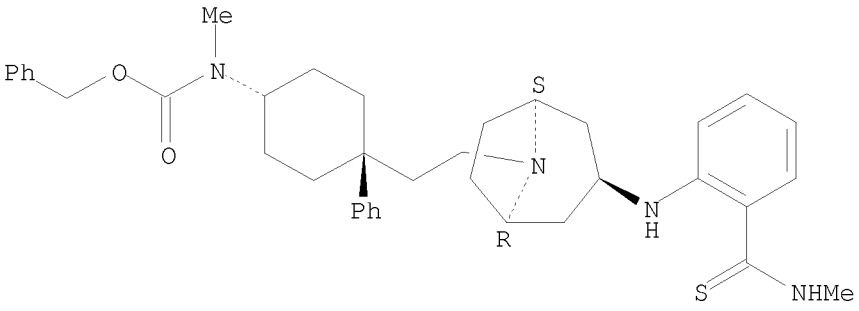
RN 714968-06-6 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-(2-methyl-1H-benzimidazol-1-yl)-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



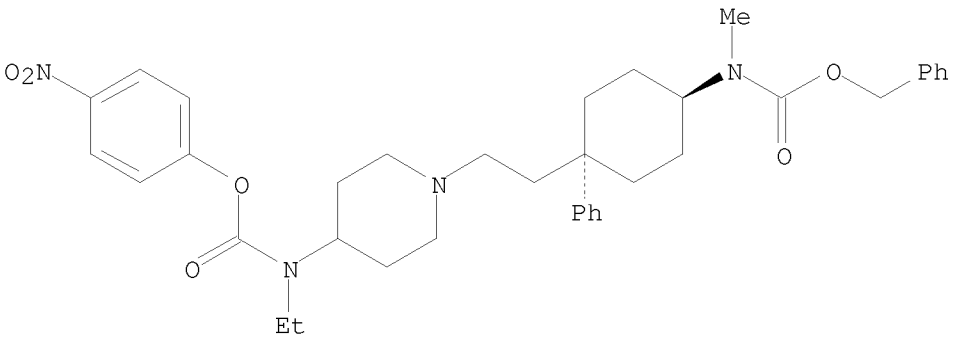
RN 714968-07-7 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[(3-endo)-3-[[2-[(methylamino)thioxomethyl]phenyl]amino]-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



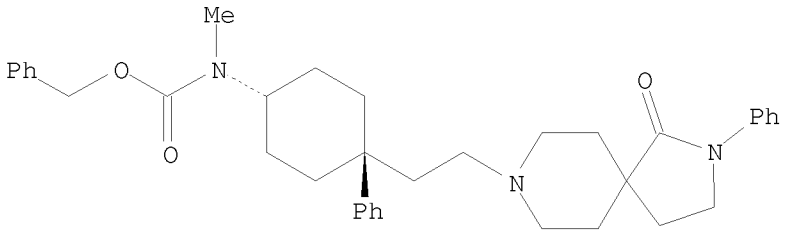
RN 714968-08-8 CAPLUS
CN Carbamic acid, ethyl[1-[2-[trans-4-[methyl[(phenylmethoxy)carbonyl]amino]-1-phenylcyclohexyl]ethyl]-4-piperidinyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



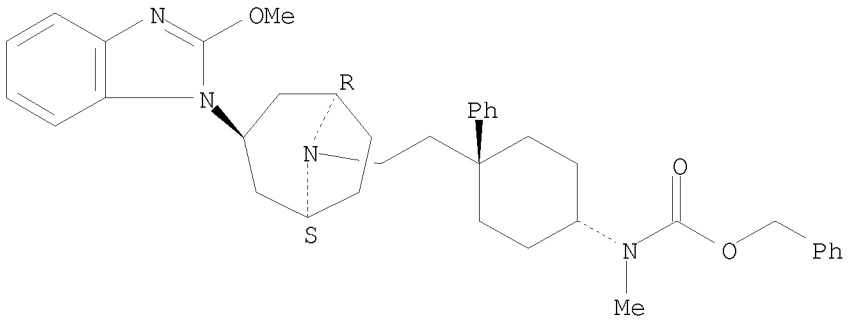
RN 714968-09-9 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-(1-oxo-2-phenyl-2,8-diazaspiro[4.5]dec-8-yl)ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



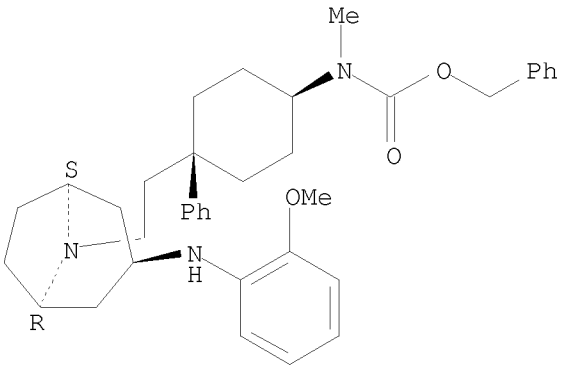
RN 714968-10-2 CAPLUS
CN Carbamic acid, [trans-4-[2-[(3-endo)-3-(2-methoxy-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



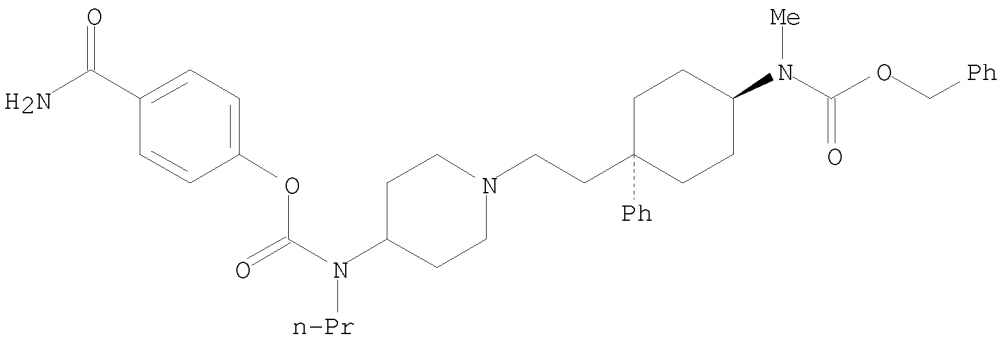
RN 714968-11-3 CAPLUS
CN Carbamic acid, [cis-4-[2-[(3-endo)-3-[(2-methoxyphenyl)amino]-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



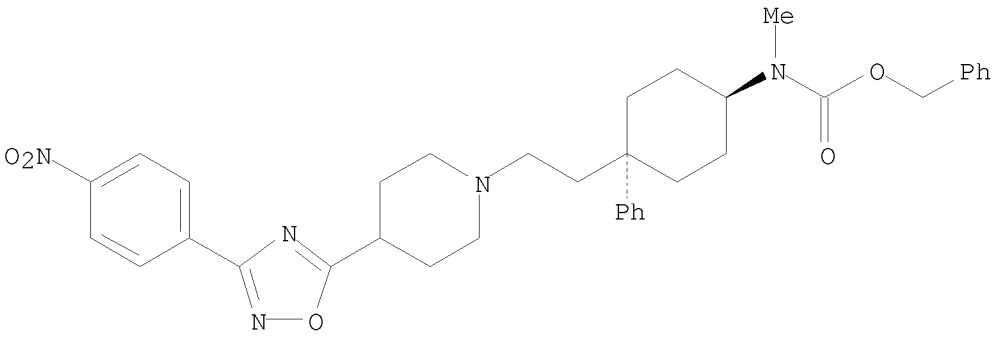
RN 714968-12-4 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[[[4-(aminocarbonyl)phenoxy]carbonyl]propylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



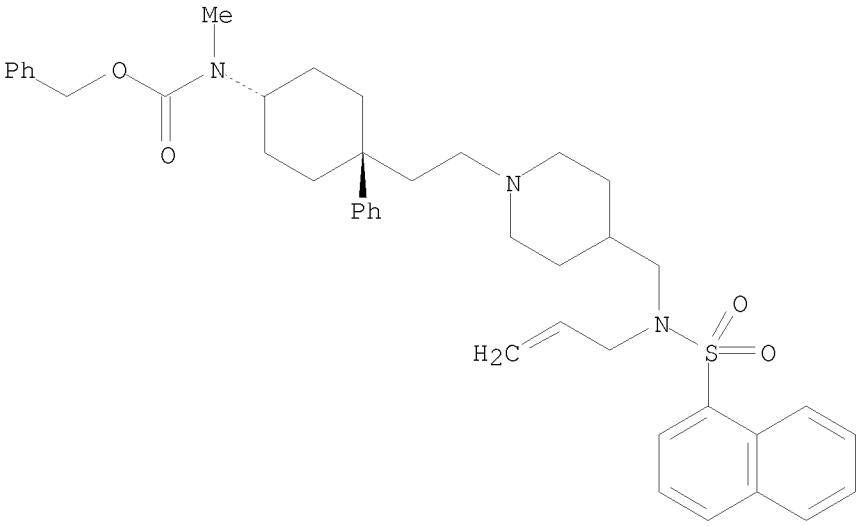
RN 714968-13-5 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[3-(4-nitrophenyl)-1,2,4-oxadiazol-5-yl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



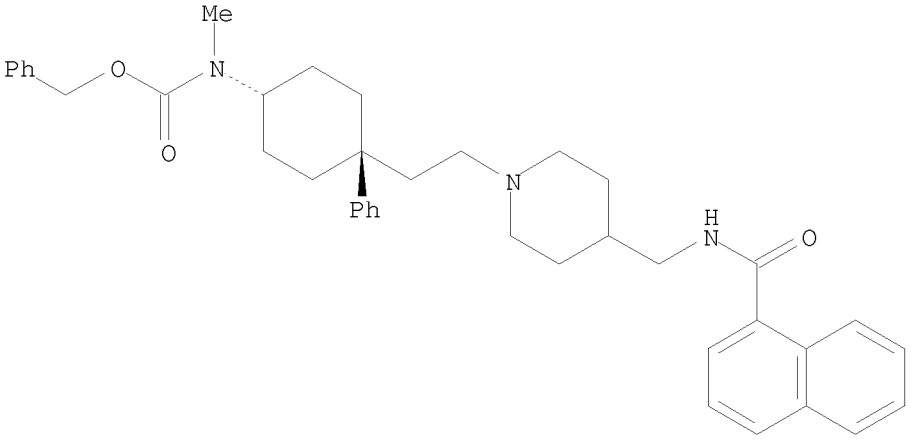
RN 714968-14-6 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylsulfonyl)-2-propenylamino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



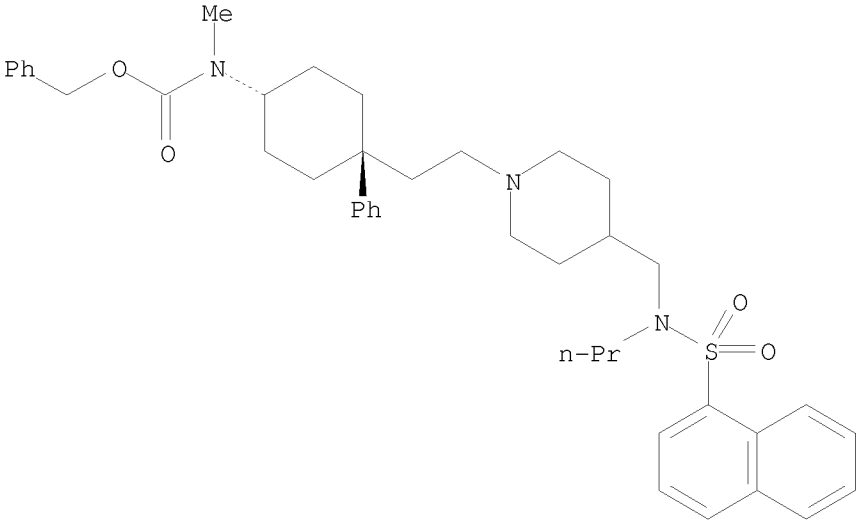
RN 714968-15-7 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylcarbonyl)amino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



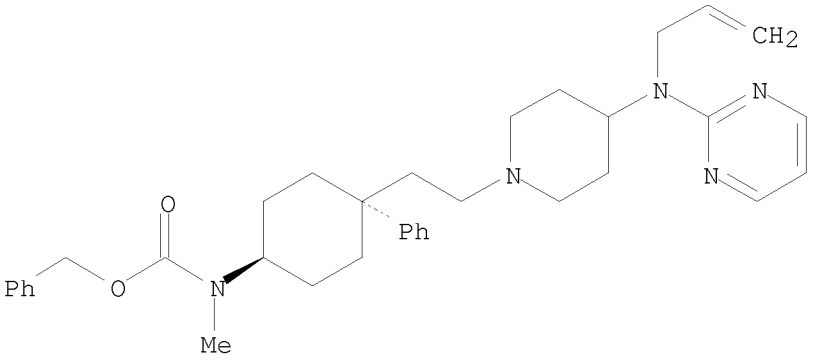
RN 714968-16-8 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[4-[[(1-naphthalenylsulfonyl)propylamino]methyl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



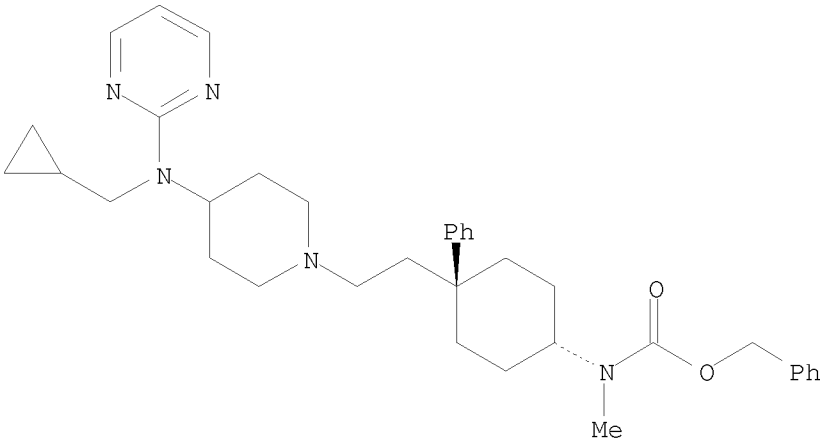
RN 714968-17-9 CAPLUS
CN Carbamic acid, methyl[trans-4-phenyl-4-[2-[4-(2-propenyl-2-pyrimidinylamino)-1-piperidinyl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



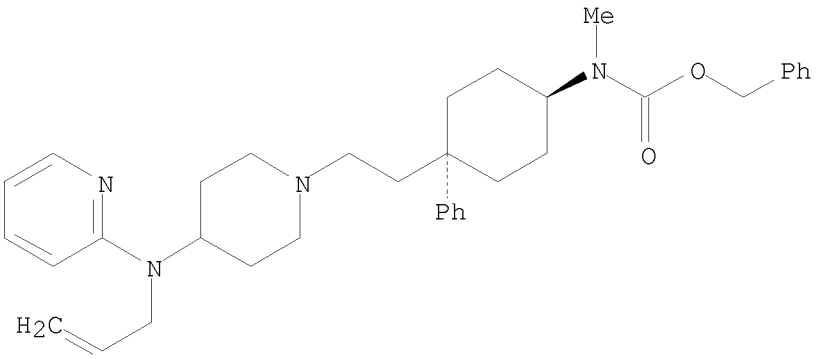
RN 714968-18-0 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(cyclopropylmethyl)-2-pyrimidinylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



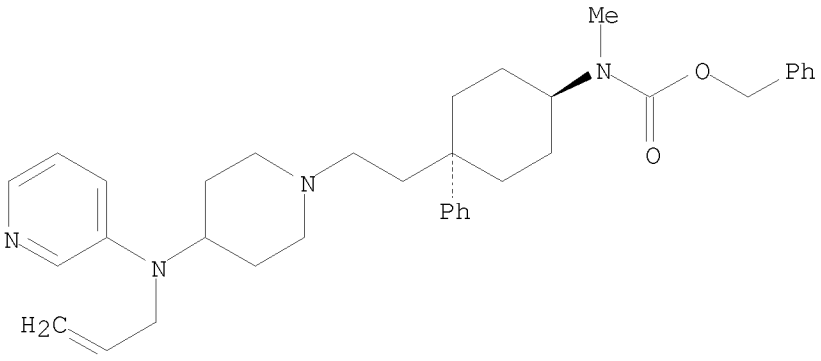
RN 714968-19-1 CAPLUS
CN Carbamic acid, methyl[trans-4-phenyl-4-[2-[4-(2-propenyl-2-pyridinylamino)-1-piperidinyl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



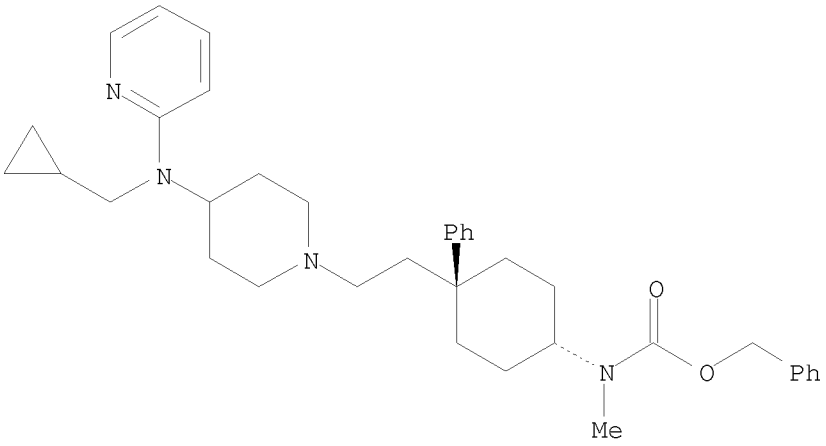
RN 714968-20-4 CAPLUS
CN Carbamic acid, methyl[trans-4-phenyl-4-[2-[4-(2-propenyl-3-pyridinylamino)-1-piperidinyl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



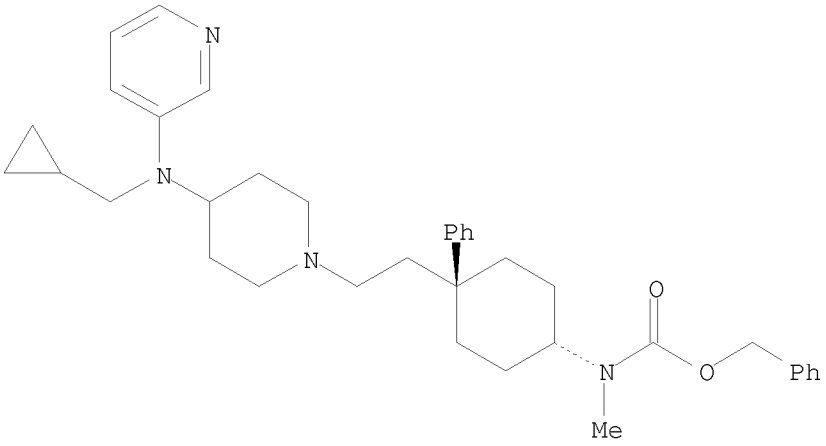
RN 714968-21-5 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(cyclopropylmethyl)-2-pyridinylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



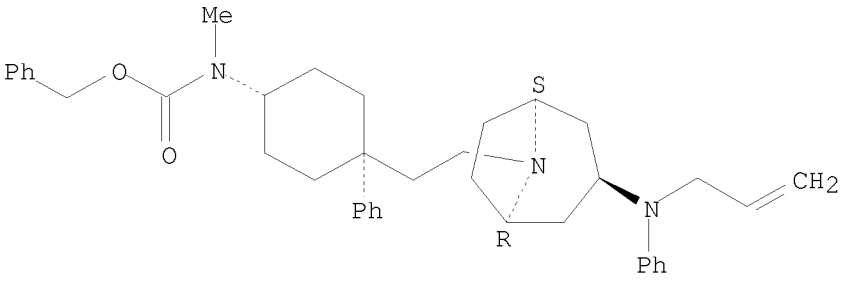
RN 714968-22-6 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(cyclopropylmethyl)-3-pyridinylamino]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



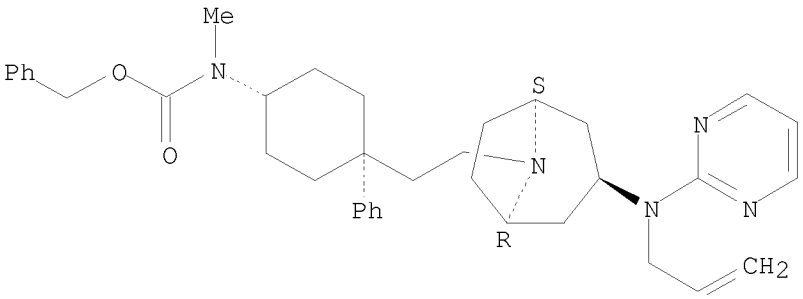
RN 714968-23-7 CAPLUS
CN Carbamic acid, methyl[cis-4-phenyl-4-[2-[(3-endo)-3-(phenyl-2-propenylamino)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



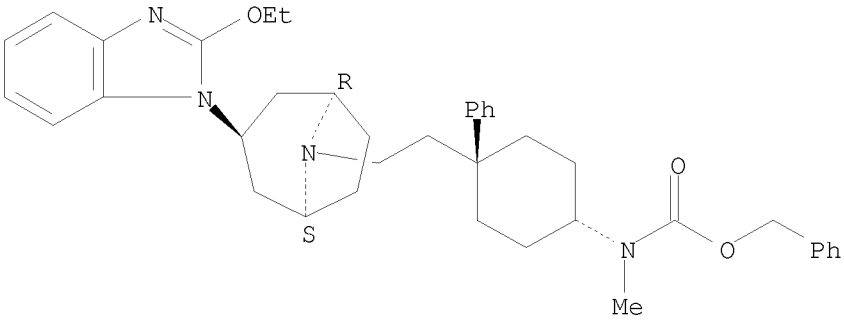
RN 714968-24-8 CAPLUS
CN Carbamic acid, methyl[cis-4-phenyl-4-[2-[(3-endo)-3-(2-propenyl-2-pyrimidinylamino)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 714968-25-9 CAPLUS
CN Carbamic acid, [trans-4-[2-[(3-endo)-3-(2-ethoxy-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

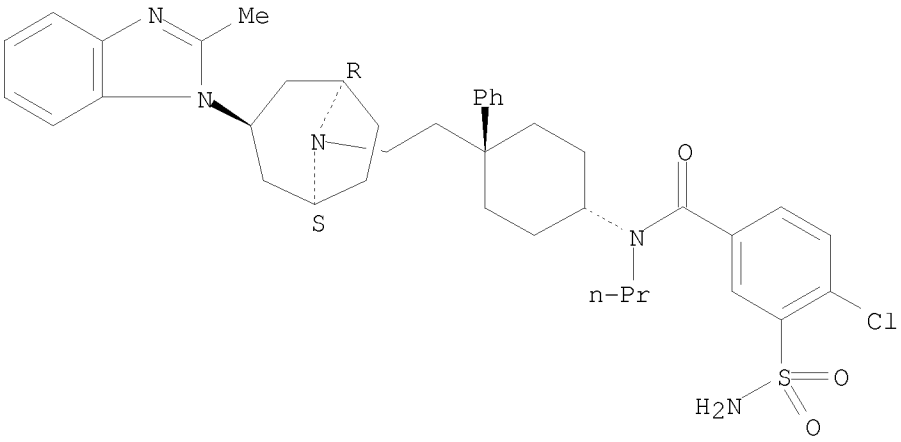
Relative stereochemistry.



RN 714968-27-1 CAPLUS

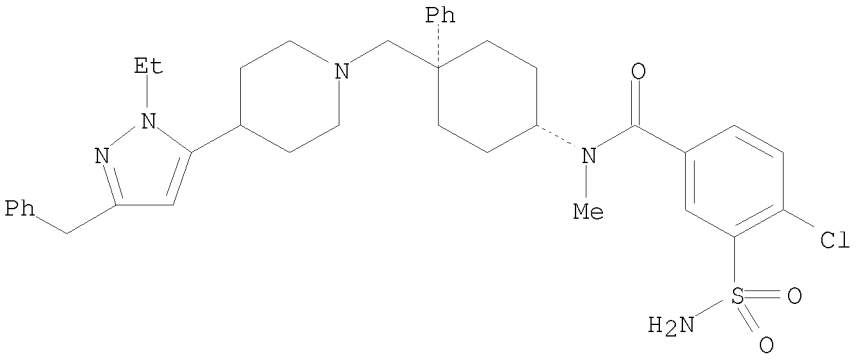
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-N-propyl- (CA INDEX NAME)

Relative stereochemistry.



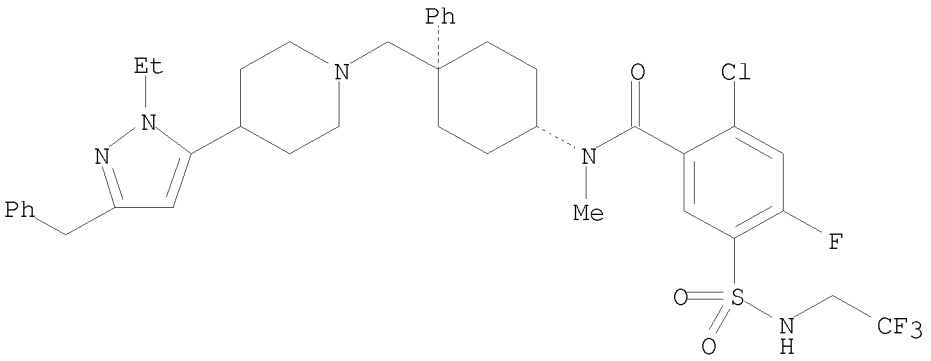
RN 714968-28-2 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[trans-4-[[4-[1-ethyl-3-(phenylmethyl)-1H-pyrazol-5-yl]-1-piperidinyl]methyl]-4-phenylcyclohexyl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.



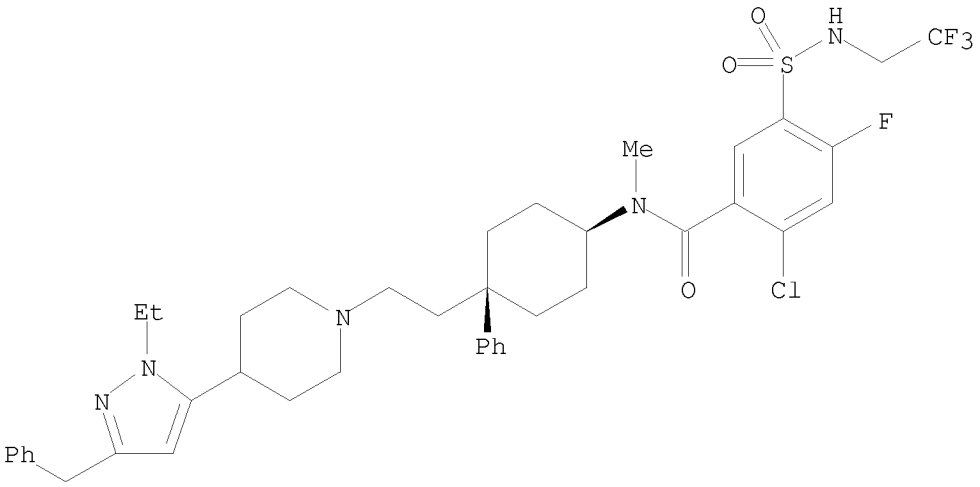
RN 714968-29-3 CAPLUS
CN Benzamide, 2-chloro-N-[trans-4-[[4-[1-ethyl-3-(phenylmethyl)-1H-pyrazol-5-yl]-1-piperidinyl]methyl]-4-phenylcyclohexyl]-4-fluoro-N-methyl-5-[[(2,2,2-trifluoroethyl)amino]sulfonyl]- (CA INDEX NAME)

Relative stereochemistry.



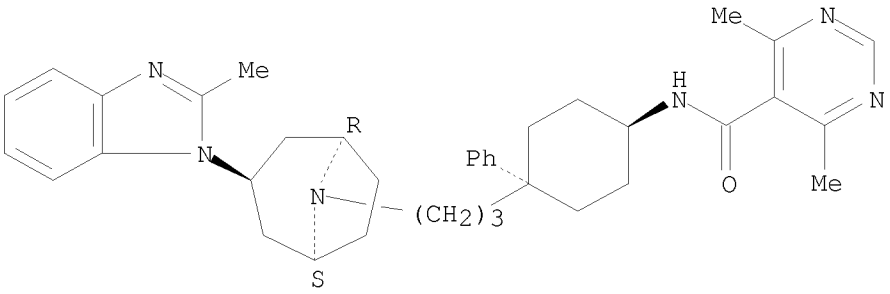
RN 714968-30-6 CAPLUS
CN Benzamide, 2-chloro-N-[cis-4-[2-[4-[1-ethyl-3-(phenylmethyl)-1H-pyrazol-5-yl]-1-piperidinyl]ethyl]-4-phenylcyclohexyl]-4-fluoro-N-methyl-5-[[(2,2,2-trifluoroethyl)amino]sulfonyl]- (CA INDEX NAME)

Relative stereochemistry.



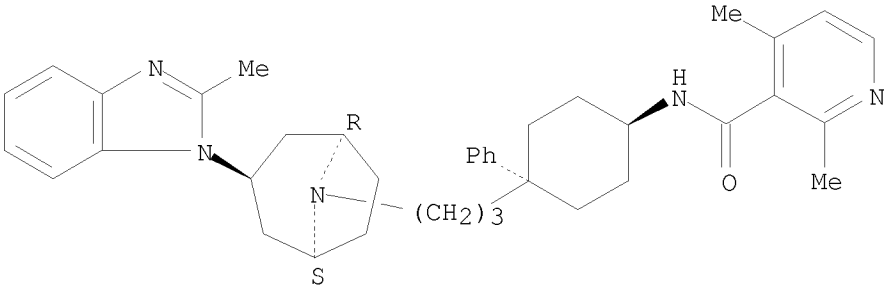
RN 714968-35-1 CAPLUS
CN 5-Pyrimidinecarboxamide, 4,6-dimethyl-N-[trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



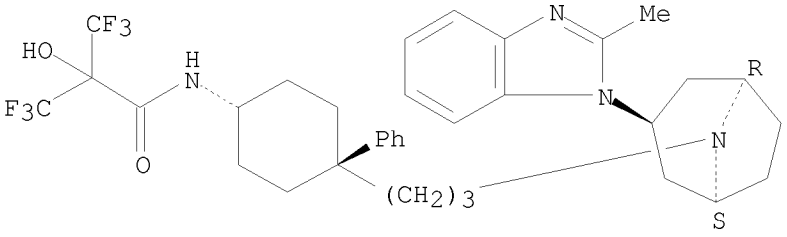
RN 714968-36-2 CAPLUS
CN 3-Pyridinecarboxamide, 2,4-dimethyl-N-[trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



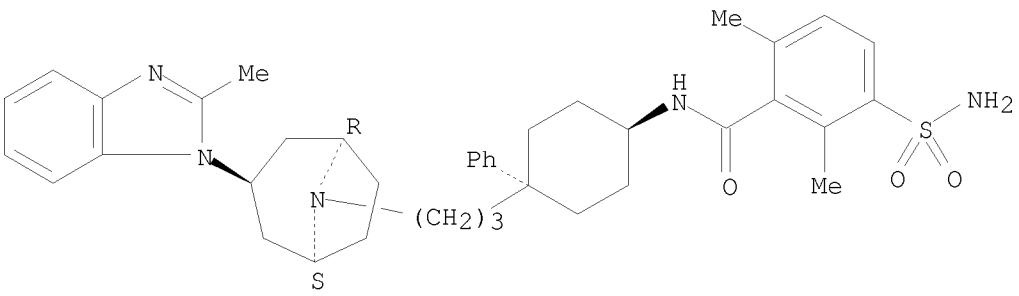
RN 714968-37-3 CAPLUS
CN Propanamide, 3,3,3-trifluoro-2-hydroxy-N-[trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl]-2-(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



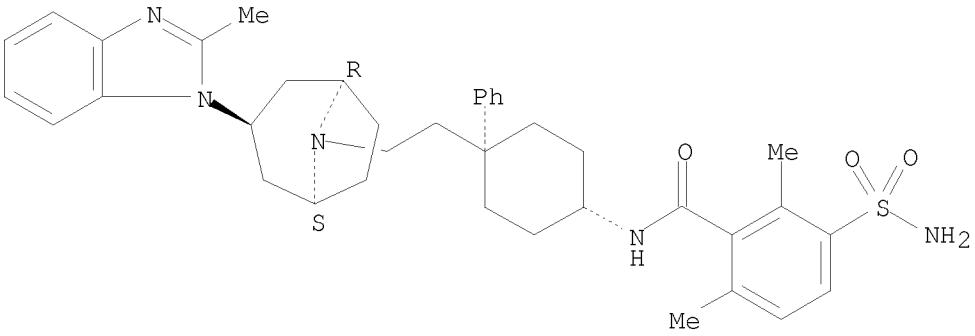
RN 714968-38-4 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-2,6-dimethyl-N-[trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



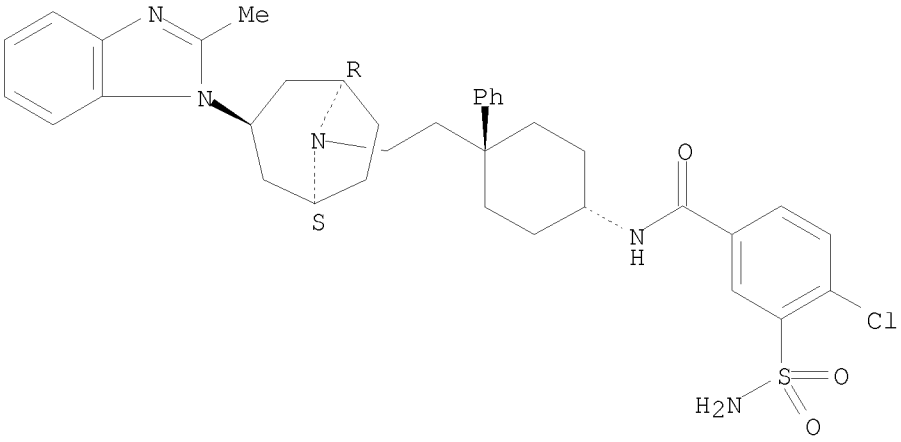
RN 716343-89-4 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-2,6-dimethyl-N-[cis-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



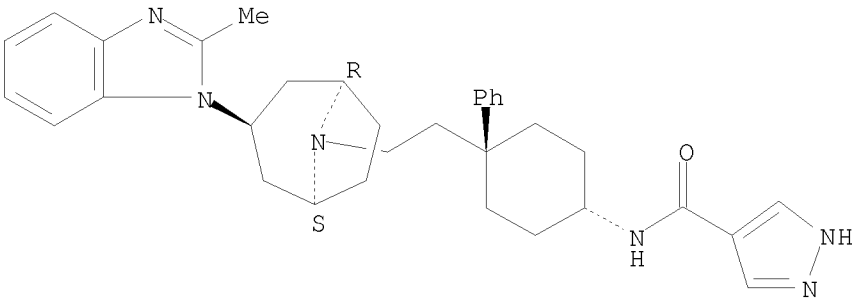
RN 716361-09-0 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



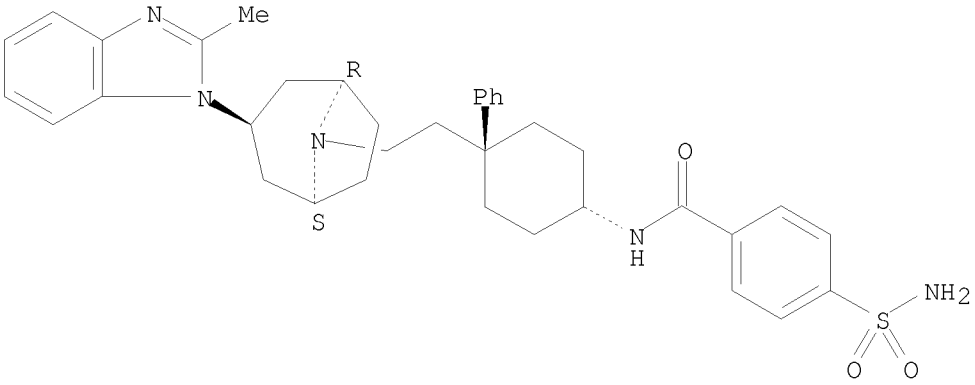
RN 716361-10-3 CAPLUS
CN 1H-Pyrazole-4-carboxamide, N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



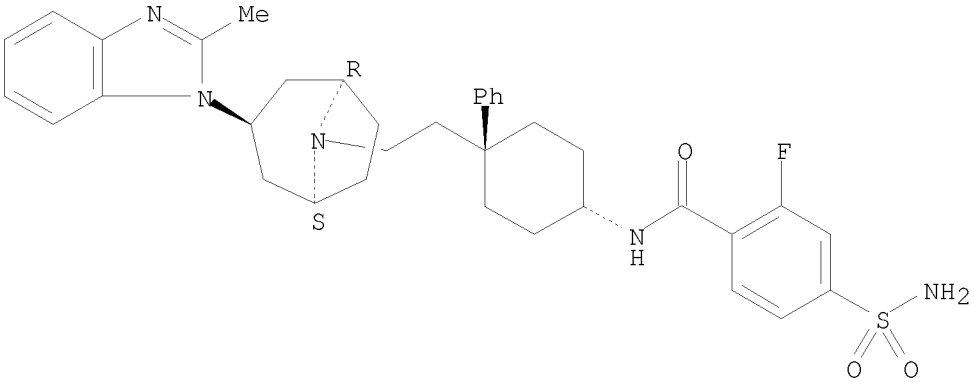
RN 716361-12-5 CAPLUS
CN Benzamide, 4-(aminosulfonyl)-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



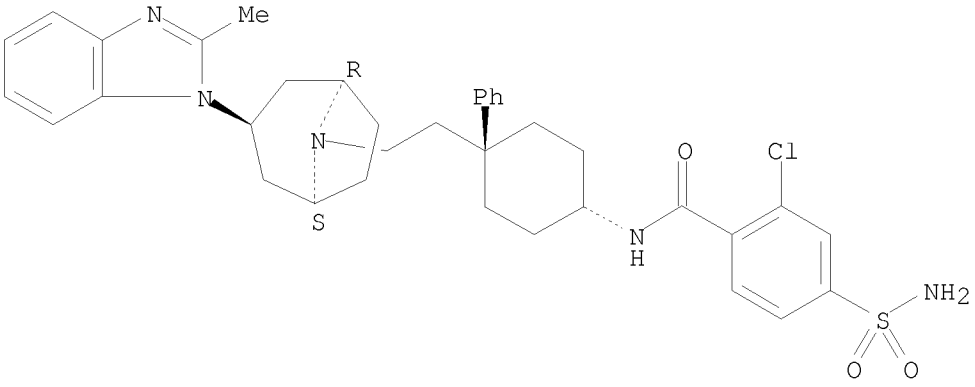
RN 716361-14-7 CAPLUS
CN Benzamide, 4-(aminosulfonyl)-2-fluoro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



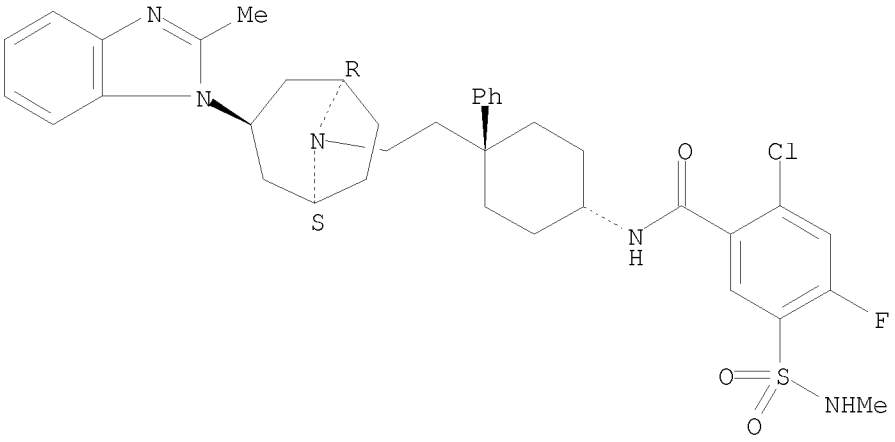
RN 716361-16-9 CAPLUS
CN Benzamide, 4-(aminosulfonyl)-2-chloro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



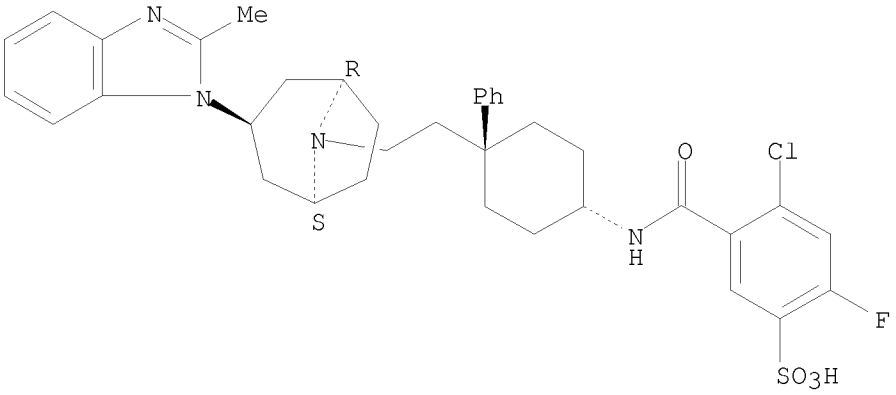
RN 716361-18-1 CAPLUS
CN Benzamide, 2-chloro-4-fluoro-5-[(methylamino)sulfonyl]-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



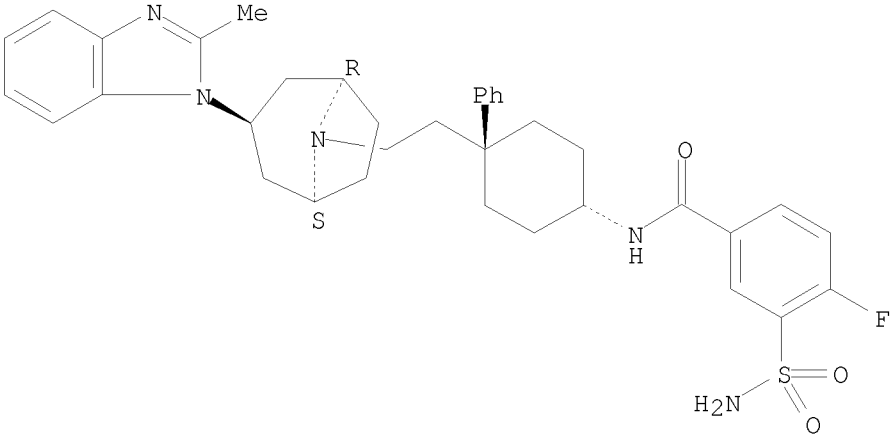
RN 716361-20-5 CAPLUS
CN Benzenesulfonic acid, 4-chloro-2-fluoro-5-[[[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]amino]carbonyl]- (CA INDEX NAME)

Relative stereochemistry.



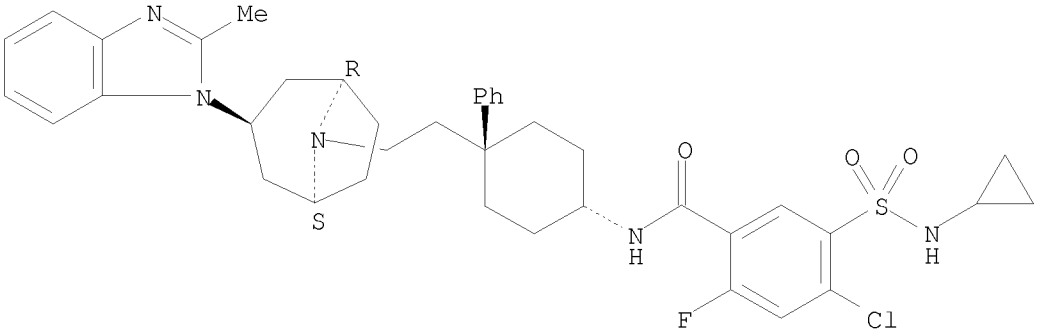
RN 716361-22-7 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-fluoro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



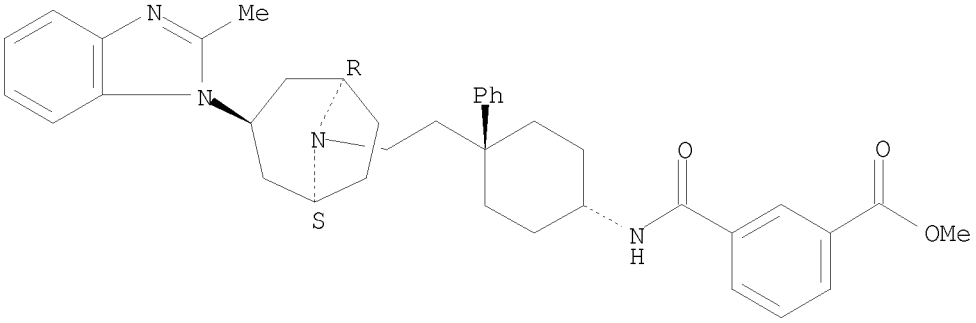
RN 716361-24-9 CAPLUS
CN Benzamide, 4-chloro-5-[(cyclopropylamino)sulfonyl]-2-fluoro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



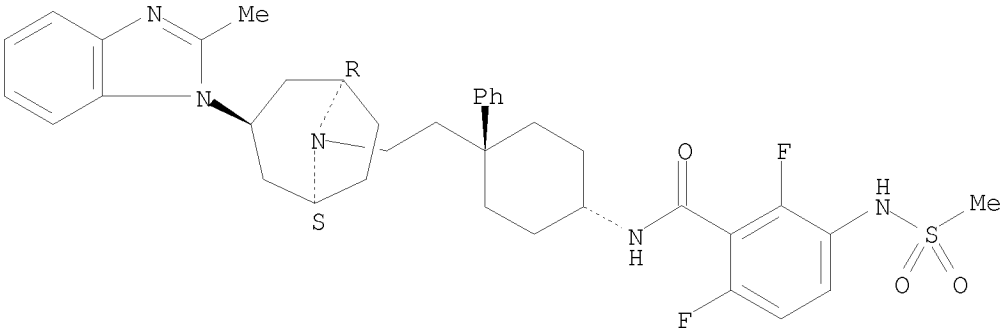
RN 716361-26-1 CAPLUS
CN Benzoic acid, 3-[[[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Relative stereochemistry.



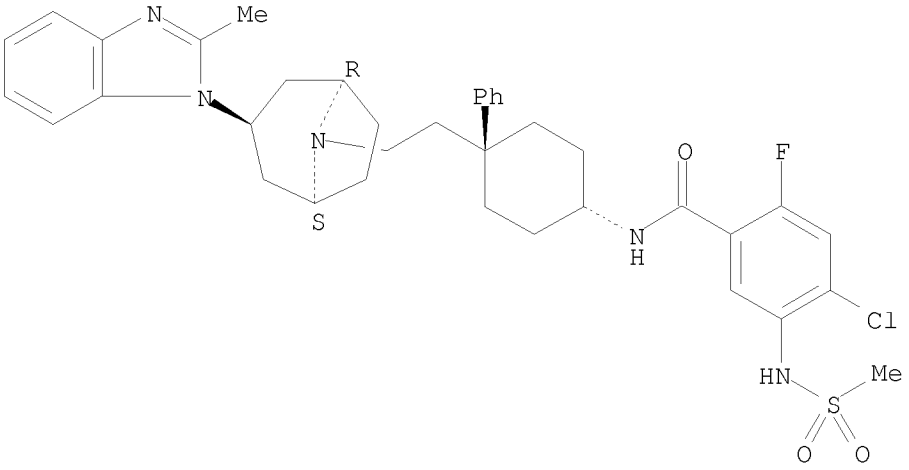
RN 716361-28-3 CAPLUS
CN Benzamide, 2,6-difluoro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-3-[(methylsulfonyl)amino]- (CA INDEX NAME)

Relative stereochemistry.



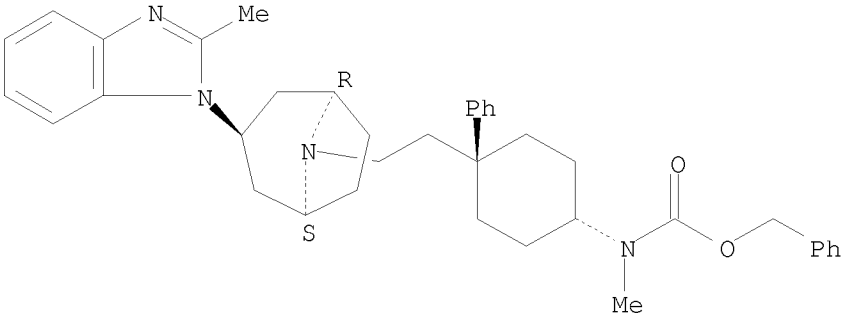
RN 716361-30-7 CAPLUS
CN Benzamide, 4-chloro-2-fluoro-N-[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-5-[(methylsulfonyl)amino]- (CA INDEX NAME)

Relative stereochemistry.



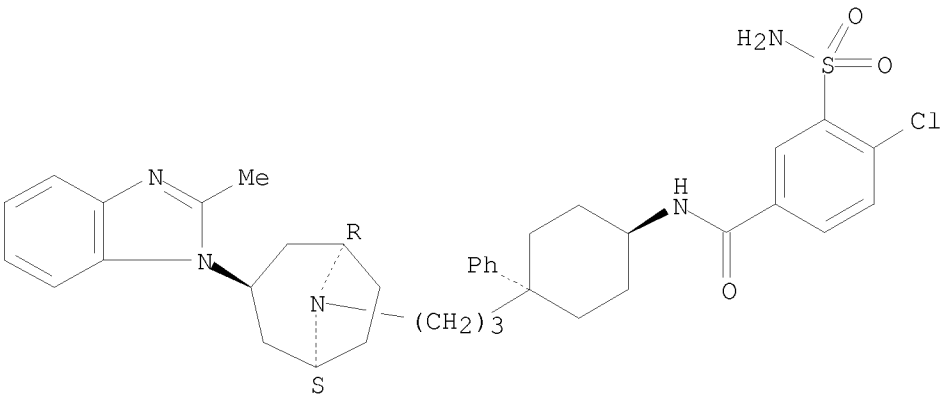
RN 716361-32-9 CAPLUS
CN Carbamic acid, methyl[trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 716361-34-1 CAPLUS
CN Benzamide, 3-(aminosulfonyl)-4-chloro-N-[trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

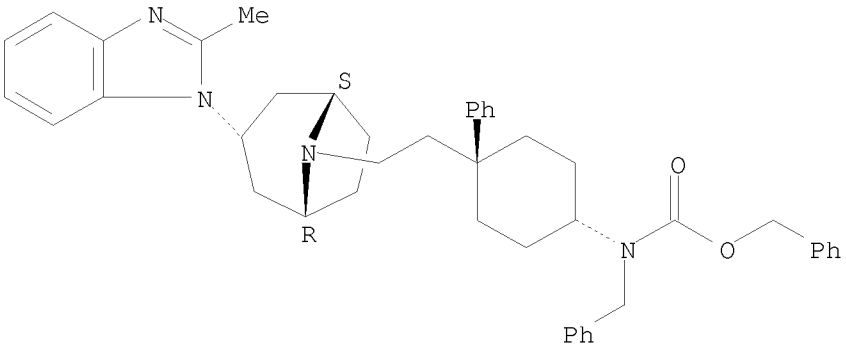


IT 714967-84-7P 714968-33-9P 714968-40-8P
716343-88-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclylalkyl substituted cyclohexanes derivs. as CCR5 antagonists)

RN 714967-84-7 CAPLUS

CN Carbamic acid, [trans-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

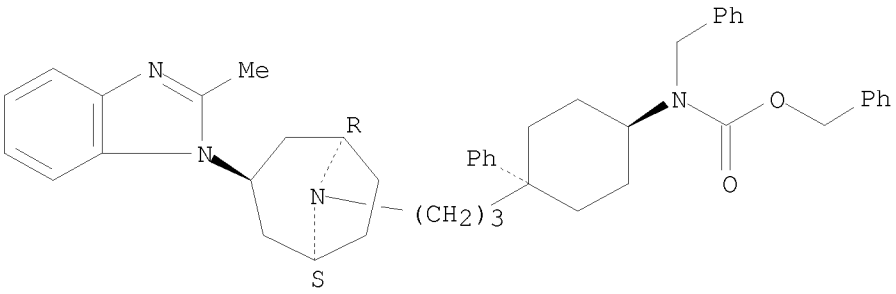
Relative stereochemistry.



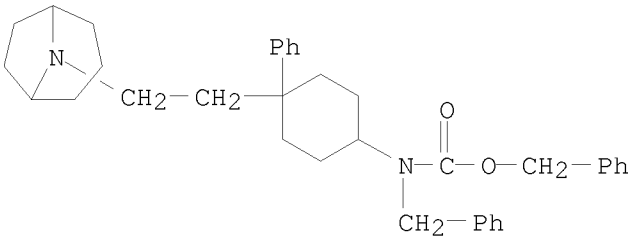
RN 714968-33-9 CAPLUS

CN Carbamic acid, [trans-4-[3-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

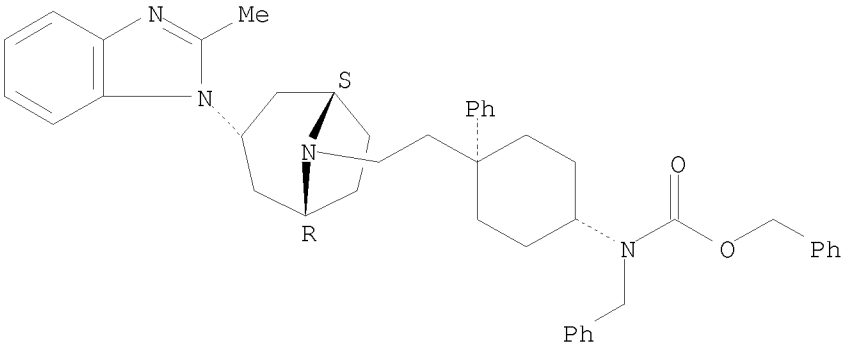


RN 714968-40-8 CAPLUS
CN Carbamic acid, [4-[2-(8-azabicyclo[3.2.1]oct-8-yl)ethyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 716343-88-3 CAPLUS
CN Carbamic acid, [cis-4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenylcyclohexyl](phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:310829 CAPLUS <<LOGINID::20081022>>

DOCUMENT NUMBER: 140:303552
TITLE: Preparation of β-amino acid derivatives as inhibitors of matrix metalloproteases and TNF-α
INVENTOR(S): Duan, Jingwu; King, Bryan W.; Decicco, Carl; Maduskuie, Thomas P.; Voss, Mathew E.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 150 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040072802	A1	20040415	US 2002-267207	20021009 <--
PRIORITY APPLN. INFO.:			US 2002-267207	20021009 <--

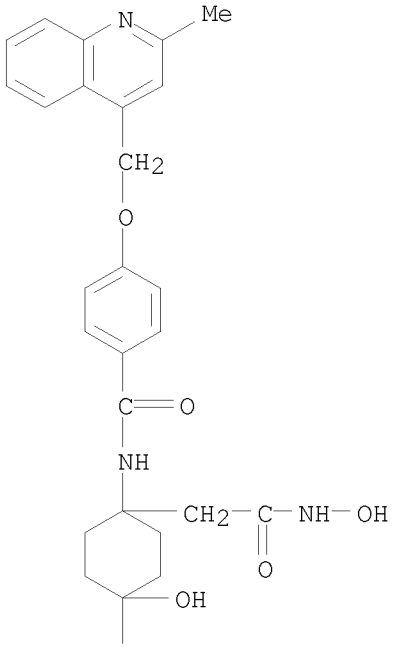
OTHER SOURCE(S): MARPAT 140:303552

AB Novel β-amino acid derivs. A-CR3R4aCR2R4NR1CO-X-Z-Ua-Xa-Ya-Za [A = CO2H, SH, CH2SH, S(O)Ra:NH (Ra = H, alkyl), P(O)(OH)2, etc.; X, Xa is absent or alkylene, alkenylene or alkynylene; Z is absent or substituted C3-13 carbocycle or 5-14 membered heterocycle; Ua is absent or O, NRa1 [Ra1 = H, (un)substituted alkyl, alkenyl or alkynyl; Ra and Ra1 may form a ring], CO, CO2, O2C, CONRa1, S(O)p (p = 0-2), etc.; Ya is absent or O, NRa1, S(O)p or CO; Za is H, substituted C3-13 carbocycle or 5-14 membered heterocycle; R1 is H, alkyl, Ph, benzyl; R2 is Q (Q is H, substituted carbocycle or heterocycle), alkylene-Q, (CRaRa1)r1O(CRaRa1)r-Q (r, r1 = 0-4), (CRaRa1)r1NRa(CRaRa1)r-Q, etc.; R3 = Q1 (Q1 is any group given for Q), alkylene-Q1, (CRaRa1)r1O(CRaRa1)r-Q1, (CRaRa1)r1NRa(CRaRa1)r-Q1, etc.; R4, R4a = H, substituted alkyl, alkenyl or alkynyl; alternatively R1 and R2, R1 and R3, R3 and R4a may form rings (with provisos)] or a stereoisomer or pharmaceutically acceptable salt were prepared as metalloprotease and TNF-α inhibitors. Thus, N-hydroxy-1-[[4-[(2-methyl-4-quinolinyl)methoxy]phenyl]acetyl]-3-azetidinecarboxamide was prepared by a multistep procedure involving reactions of Me 4-hydroxyphenylacetate, 2-methyl-4-quinolinylmethanol, and 3-azetidinecarboxylic acid Me ester.

IT 1055740-28-7
RL: PRPH (Prophetic)
(Preparation of β-amino acid derivatives as inhibitors of matrix metalloproteases and TNF-α)

RN 1055740-28-7 CAPLUS
CN Benzamide, N-[4-hydroxy-1-[2-(hydroxyamino)-2-oxoethyl]-4-[2-(1-piperidinyl)ethyl]cyclohexyl]-4-[(2-methyl-4-quinolinyl)methoxy]- (CA INDEX NAME)

PAGE 1-A



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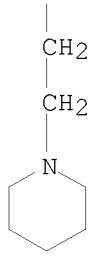

L18 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:656589 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 139:197496
TITLE: Preparation of triazolopyridiazinediones as tryptase inhibitors and β-sheet mimetics
INVENTOR(S): Ogbu, Cyprian O.; Kim, Hwa-Ok; Blaskovich, Mark A.
PATENT ASSIGNEE(S): Molecumetics Ltd., USA
SOURCE: PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2003068237	A1	20030821	WO 2003-US4993		20030214	<--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW						
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
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US 20040014763	A1	20040122	US 2003-367575		20030214	<--
US 7053214	B2	20060530				
EP 1482941	A1	20041208	EP 2003-716084		20030214	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK						
CN 1642550	A	20050720	CN 2003-806471		20030214	<--
JP 2005526722	T	20050908	JP 2003-567419		20030214	<--
IN 2004KN01283	A	20060714	IN 2004-KN1283		20040901	<--
US 20060084653	A1	20060420	US 2005-295833		20051206	<--
PRIORITY APPLN. INFO.:			US 2002-357261P	P	20020214	<--
			US 2003-367575	A3	20030214	
			WO 2003-US4993	W	20030214	

OTHER SOURCE(S): MARPAT 139:197496
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

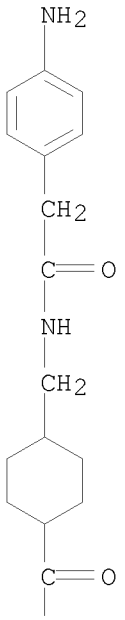
AB Title compds. I [A, A1 = N, CH; A2 = (CH2)1-3; B = CR1NHZ, NZ, CR1Z; X = (un)substituted divalent heterocycle; Y, Z = rest of the mol.; R1-R5 = amino acid-derived side chain] and some unsatd. derivs. were prepared by solid-phase synthesis. I are tryptase antagonists for use in treating diseases, such as asthma, pulmonary fibrosis, interstitial pneumonia, nephritis, hepatic fibrosis, hepatitis, hepatic cirrhosis, scleroderma, psoriasis, atopic dermatitis, chronic rheumatoid arthritis, influenza, Crohn's disease, ulcerative colitis, inflammatory bowel disease, nasal allergy, atherosclerosis, or post-operative ileus. Thus, the triazolopyridazine II was prepared from the piperidine fragment III by solid-phase synthesis. II inhibits human lung tryptase by ≥ 70% at 400 nM.

IT 583868-56-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of triazolopyridiazinediones as tryptase inhibitors and β-sheet mimetics)

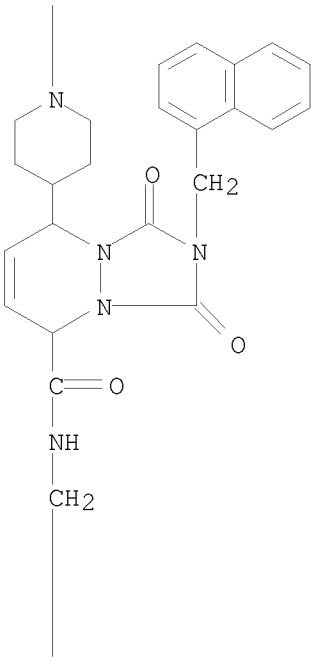
RN 583868-56-8 CAPLUS

CN 1H-[1,2,4]Triazolo[1,2-a]pyridazine-5-carboxamide, N-[[4-(aminomethyl)phenyl]methyl]-8-[1-[[4-[[[2-(4-aminophenyl)acetyl]amino]methyl]cyclohexyl]carbonyl]-4-piperidinyl]-2,3,5,8-tetrahydro-2-(1-naphthalenylmethyl)-1,3-dioxo- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



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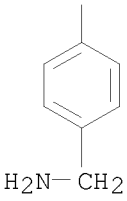
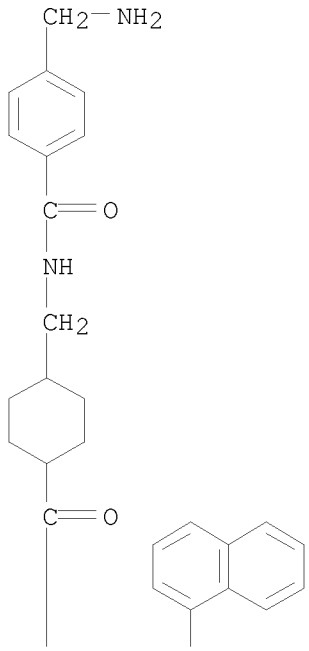


IT 583868-64-8P 583868-78-4P 583868-87-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of triazolopyridiazinediones as tryptase inhibitors and β-sheet mimetics)
RN 583868-64-8 CAPLUS
CN 1H-[1,2,4]Triazolo[1,2-a]pyridazine-5-carboxamide, 8-[1-[[4-[[[4-(aminomethyl)benzoyl]amino]methyl]cyclohexyl]carbonyl]-4-piperidinyl]-N-[[4-(aminomethyl)phenyl]methyl]-2,3,5,8-tetrahydro-2-(1-naphthalenylmethyl)-1,3-dioxo- (CA INDEX NAME)

PAGE 1-A



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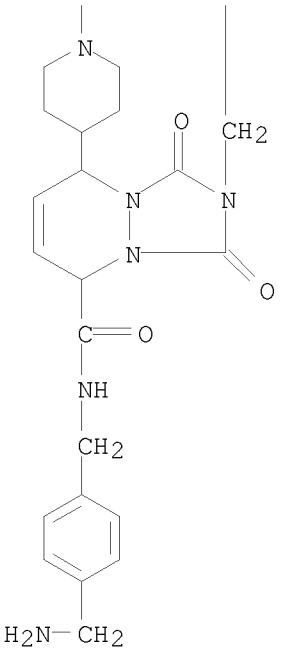
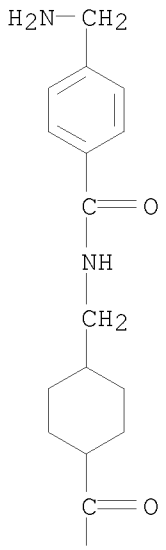


RN 583868-78-4 CAPLUS
CN 1H-[1,2,4]Triazolo[1,2-a]pyridazine-5-carboxamide, 2-[[3-[(aminoiminomethyl)amino]phenyl]methyl]-8-[1-[[4-[[[4-(aminomethyl)benzoyl]amino]methyl]cyclohexyl]carbonyl]-4-piperidinyl]-N-[[4-(aminomethyl)phenyl]methyl]-2,3,5,8-tetrahydro-1,3-dioxo- (CA INDEX NAME)

PAGE 1-A



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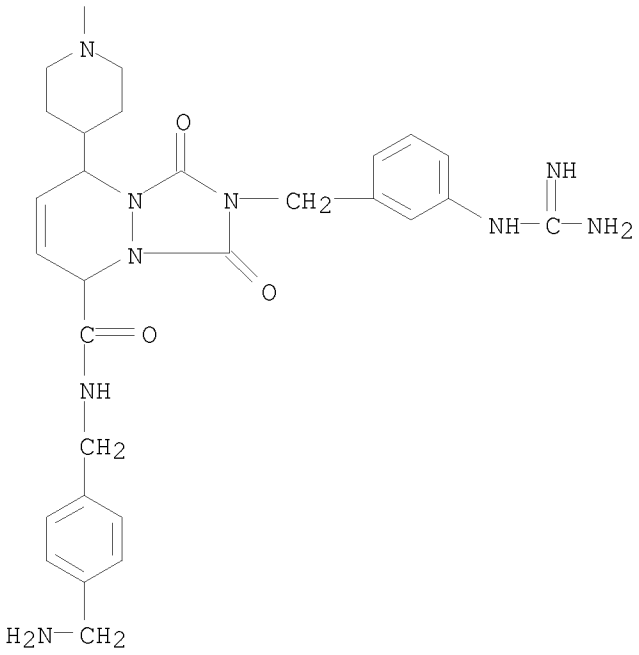
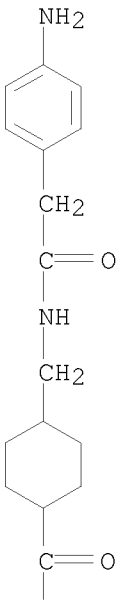


RN 583868-87-5 CAPLUS
CN 1H-[1,2,4]Triazolo[1,2-a]pyridazine-5-carboxamide, 2-[[3-[(aminoiminomethyl)amino]phenyl]methyl]-N-[[4-(aminomethyl)phenyl]methyl]-8-[1-[[4-[[[2-(4-aminophenyl)acetyl]amino]methyl]cyclohexyl]carbonyl]-4-piperidinyl]-2,3,5,8-tetrahydro-1,3-dioxo- (CA INDEX NAME)

PAGE 1-A



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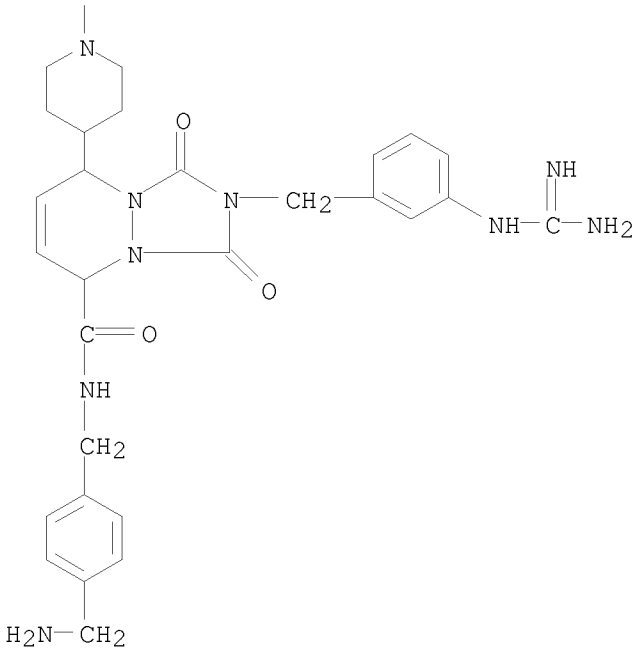
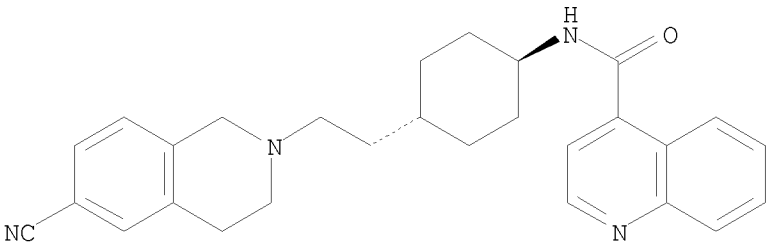


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:645541 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 139:143837
TITLE: Dopamine D3 receptor antagonism inhibits cocaine-seeking and cocaine-enhanced brain reward in rats
AUTHOR(S): Vorel, Stanislav R.; Ashby, Charles R., Jr.; Paul, Mousumi; Liu, Xinhe; Hayes, Robert; Hagan, Jim J.; Middlemiss, Derek N.; Stemp, Geoffrey; Gardner, Eliot L.
CORPORATE SOURCE: Intramural Research Program, National Institute on Drug Abuse, Baltimore, MD, 21224, USA
SOURCE: Journal of Neuroscience (2002), 22(21), 9595-9603
CODEN: JNRSDS; ISSN: 0270-6474
PUBLISHER: Society for Neuroscience
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dopamine D3 receptor is preferentially localized to the mesocorticolimbic dopaminergic system and has been hypothesized to play a role in cocaine addiction. To study the involvement of the D3 receptor in brain mechanisms and behaviors commonly assumed to be involved in the addicting properties of cocaine, the potent and selective D3 receptor antagonist SB-277011-A was administered to laboratory rats, and the following measures were assessed: (1) cocaine-enhanced elec. brain-stimulation reward, (2) cocaine-induced conditioned place preference, and (3) cocaine-triggered reinstatement of cocaine seeking behavior. Systemic injections of SB-277011-A were found to (1) block enhancement of elec. brain stimulation reward by cocaine, (2) dose-dependently attenuate cocaine-induced conditioned place preference, and (3) dose-dependently attenuate cocaine-triggered reinstatement of cocaine seeking behavior. Thus, D3 receptor blockade attenuates both the rewarding effects of cocaine and cocaine-induced drug-seeking behavior. These data suggest an important role for D3 receptors in mediating the addictive properties of cocaine and suggest that blockade of dopamine D3 receptors may constitute a new and useful target for prospective pharmacotherapies for cocaine addiction.
IT 215803-78-4, SB 277011A
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(dopamine D3 receptor antagonism inhibits cocaine-seeking and cocaine-enhanced brain reward in rats)
RN 215803-78-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:511296 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 139:85334
TITLE: Preparation of benzyl cyclic amines such as benzylpiperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Kodo, Toru; Yagi, Hideki; Dan, Akihito; Masumoto, Shuji; Kinomura, Naoya; Koyama, Koji
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 186 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003053928	A1	20030703	WO 2002-JP13043		20021212 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2002366766	A1	20030709	AU 2002-366766		20021212 <--
EP 1466901	A1	20041013	EP 2002-790747		20021212 <--
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US 20050065140	A1	20050324	US 2004-498482		20040816 <--
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			JP 2001-399453	A	20011228 <--
			JP 2002-7140	A	20020116 <--
			WO 2002-JP13043	W	20021212 <--

OTHER SOURCE(S): MARPAT 139:85334
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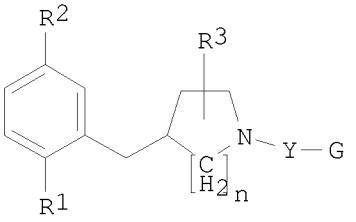

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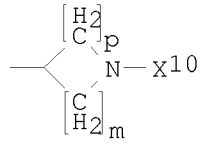
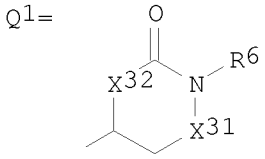
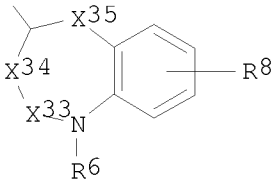






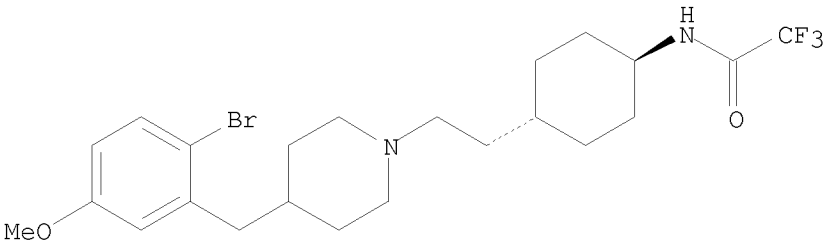
AB Disclosed is a serotonin reuptake inhibitor which contains as an active ingredient a cyclic amine represented by the formula (I) [wherein G = Q, -Z2-X20, Z3; R2 = H, halo, HO, each (un)substituted alkyl, alkoxy, or alkylthio; R3 = H, lower alkyl; Y = (un)substituted alkylene; n = 1,2,3; m = 0, 1,2,3; p = 1,2,3,4; wherein X10 = H, cycloalkyl, each (un)substituted alkyl, alkanoyl, alkanesulfonyl, alkylcarbamoyl, alkylsulfamoyl, alkoxycarbonyl, or amidino; X20 = HO, carbamoyloxy, each (un)substituted alkyl, NH2, alkoxy, or alkylcarbamoyloxy; Z2 = cycloalkane ring; Z3 = Q1, Q2; wherein X31 = a bond, CH2, CO; X32 = O, S, alkyl-(un)substituted NH; R6 = H, (un)substituted alkyl, cycloalkyl, aryl, or heteroaryl; X33 = a single bond, CH2, CO; X34 = a single bond, CH2; X35 = a single bond, CH2, O, S, alkyl-(un)substituted NH; provided that X34 and X35 are not simultaneously a single bond; R6 = H, alkyl; R8 = H, halo, alkyl, HO, (un)substituted alkoxy or alkylcarbamoyloxy], a prodrug thereof, or a pharmaceutically acceptable salt of any of these. The compds. I are selective serotonin reuptake inhibitors having an affinity for a serotonin 1A receptor. Thus, 55 mg triphosgene was added to a solution of 200 mg 3-[4-(2-bromo-5-methoxybenzyl)piperidin-1-yl]-1-cyclohexylaminopropan-2-ol and 0.083 mL Et3N in 5 m THF at room temperature and stirred for 6 h to give 100% 5-[[4-(2-bromo-5-methoxybenzyl)piperidin-1-yl]methyl]-3-cyclohexyloxazolidin-2-one. 2-[[4-(2-Bromo-5-chlorobenzyl)piperidin-1-yl]methyl]-1,2,3,4-tetrahydroquinoline dihydrochloride at 10-5 M increased by 74% the binding of [35S]GTPγS to CHO cell membrane expressing human 5-HT1A in the presence of 10 μM serotonin (5-HT).

IT 552858-48-7P 552858-49-8P 552858-51-2P
552858-53-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzyl cyclic amines such as benzylpiperidine derivs. as selective serotonin reuptake inhibitors)

RN 552858-48-7 CAPLUS

CN Acetamide, N-[trans-4-[2-[4-[(2-bromo-5-methoxyphenyl)methyl]-1-piperidinyl]ethyl]cyclohexyl]-2,2,2-trifluoro-, hydrochloride (1:1) (CA INDEX NAME)

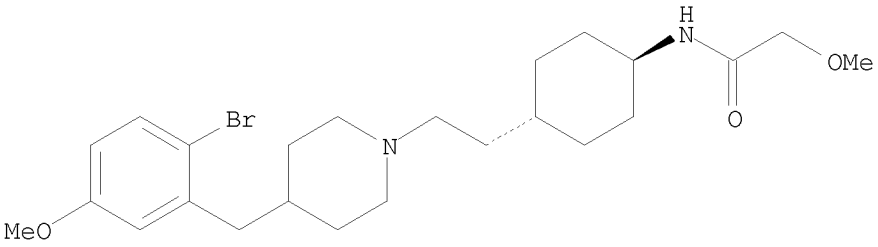
Relative stereochemistry.



● HCl

RN 552858-49-8 CAPLUS
CN Acetamide, N-[trans-4-[2-[4-[(2-bromo-5-methoxyphenyl)methyl]-1-piperidinyl]ethyl]cyclohexyl]-2-methoxy-, hydrochloride (1:1) (CA INDEX NAME)

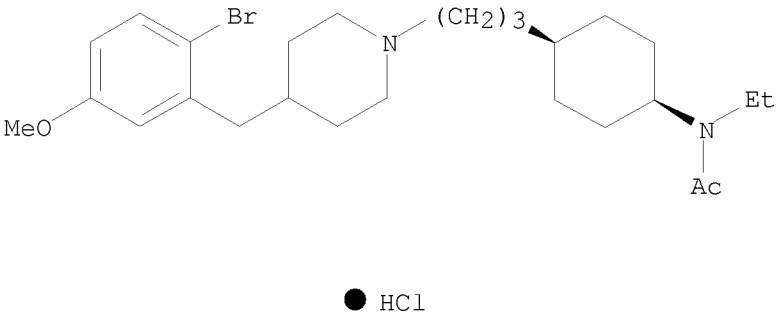
Relative stereochemistry.



● HCl

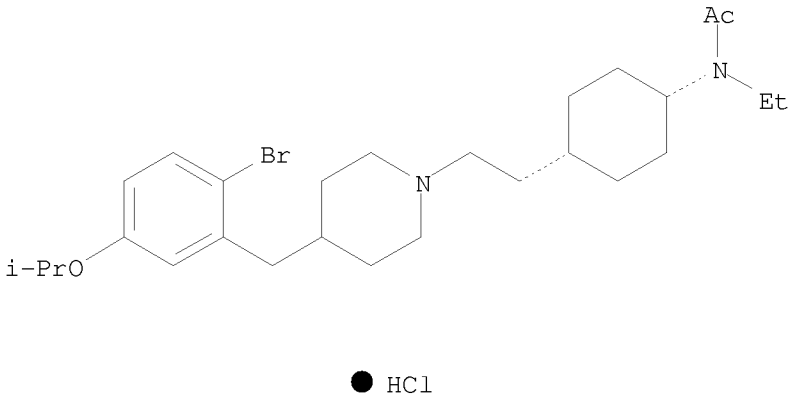
RN 552858-51-2 CAPLUS
CN Acetamide, N-[cis-4-[3-[4-[(2-bromo-5-methoxyphenyl)methyl]-1-piperidinyl]propyl]cyclohexyl]-N-ethyl-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.



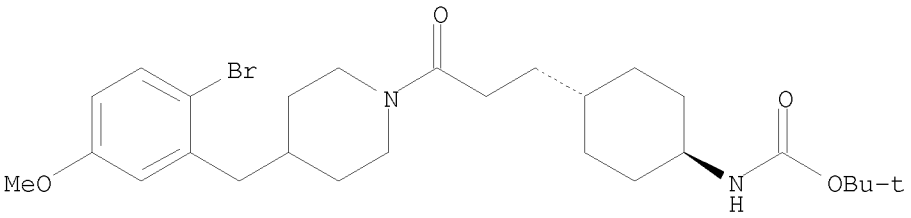
RN 552858-53-4 CAPLUS
CN Acetamide, N-[cis-4-[2-[4-[[2-bromo-5-(1-methylethoxy)phenyl]methyl]-1-piperidinyl]ethyl]cyclohexyl]-N-ethyl-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.



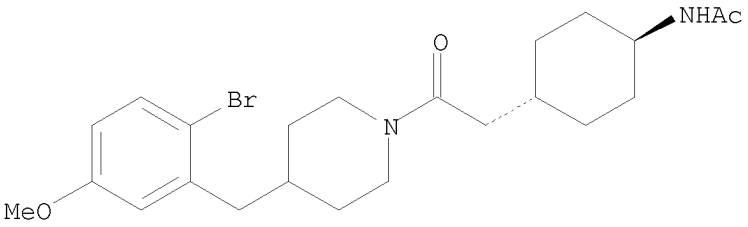
IT 552858-96-5P 552858-98-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzyl cyclic amines such as benzylpiperidine derivs. as selective serotonin reuptake inhibitors)
RN 552858-96-5 CAPLUS
CN Carbamic acid, [trans-4-[3-[4-[(2-bromo-5-methoxyphenyl)methyl]-1-piperidinyl]-3-oxopropyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 552858-98-7 CAPLUS
CN Acetamide, N-[trans-4-[2-[4-[(2-bromo-5-methoxyphenyl)methyl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:511287 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 139:85040
TITLE: Preparation of cyclohexane derivatives as inhibitors of 2,3-oxidosqualene-lanosterol cyclase
INVENTOR(S): Ackermann, Jean; Aebi, Johannes; Dehmlow, Henrietta; Hirth, Georges; Maerki, Hans-Peter; Morand, Olivier
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 114 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053919	A1	20030703	WO 2002-EP13786	20021205 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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AU 2002358096	A1	20030709	AU 2002-358096	20021205 <--
AU 2002358096	B2	20060511		
EP 1456171	A1	20040915	EP 2002-791779	20021205 <--
EP 1456171	B1	20061220		
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HU 2004002262	A2	20050228	HU 2004-2262	20021205 <--
CN 1604890	A	20050406	CN 2002-824987	20021205 <--
JP 2005513127	T	20050512	JP 2003-554636	20021205 <--
JP 4124736	B2	20080723		
RU 2288221	C2	20061127	RU 2004-121684	20021205 <--
AT 348799	T	20070115	AT 2002-791779	20021205 <--
ES 2276974	T3	20070701	ES 2002-791779	20021205 <--
US 20030199550	A1	20031023	US 2002-315770	20021210 <--
US 6953806	B2	20051011		
MX 2004PA05550	A	20040910	MX 2004-PA5550	20040608 <--
ZA 2004004547	A	20060222	ZA 2004-4547	20040608 <--
IN 2004CN01273	A	20060512	IN 2004-CN1273	20040609 <--
NO 2004002881	A	20040707	NO 2004-2881	20040707 <--
US 20050272774	A1	20051208	US 2005-176901	20050707 <--

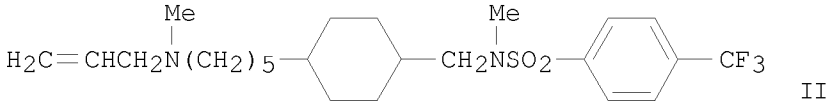
PRIORITY APPLN. INFO.:

EP 2001-129271	A	20011212 <--
WO 2002-EP13786	W	20021205 <--
US 2002-315770	A3	20021210 <--

OTHER SOURCE(S): MARPAT 139:85040

GI

I



II

AB Cyclohexanes I [V = bond, O, S, CH2, CH:CH, CH:CHCH2O, C.tplbond.C; W = CO, CO2, (un)substituted CONH, C(S)O, CSNH, SO2, SO2NH; m, n = 0-7; p = 0, 1; A1 = H, alkyl, hydroxyalkyl, alkenyl; A2 = cycloalkyl, cycloalkylalkyl, alkenyl, alkynyl, heteroaryl, (un)substituted alkyl; NA2A2 = heterocyclic; A3, A4 = H, alkyl; A3A4 = alkylene; A5-A8 = H, alkyl; A9 = H, alkyl, alkenyl, aralkyl; A10 = alkyl, cycloalkyl, aryl, aralkyl, heteroaryl, heteroarylalkyl] and their N-oxides were prepared These compds. are useful for the treatment and/or prophylaxis of diseases which are associated with

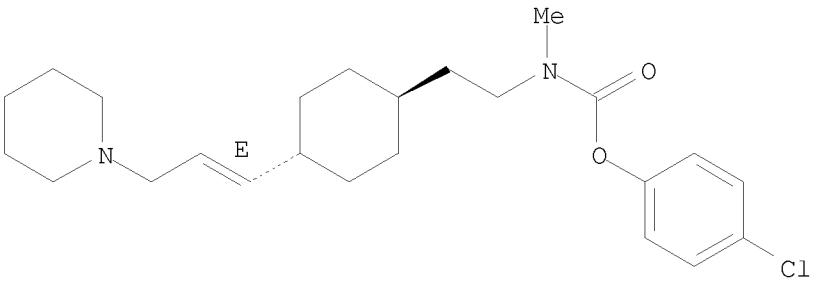
2,3-oxidosqualene-lanosterol cyclase such as hypercholesterolemia, hyperlipemia, arteriosclerosis, vascular diseases, mycoses, parasitic infections, gallstones, tumors and/or hyperproliferative disorders, and treatment and/or prophylaxis of impaired glucose tolerance and diabetes. Thus, the sulfonamide II was prepared from trans-N-tert.-butoxycarbonyl-4-hydroxymethylcyclohexylmethylamine in 8 steps.

IT 554455-77-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclohexane derivs. as inhibitors of 2,3-oxidosqualene-lanosterol cyclase)

RN 554455-77-5 CAPLUS

CN Carbamic acid, methyl[2-[trans-4-[(1E)-3-(1-piperidinyl)-1-propenyl]cyclohexyl]ethyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

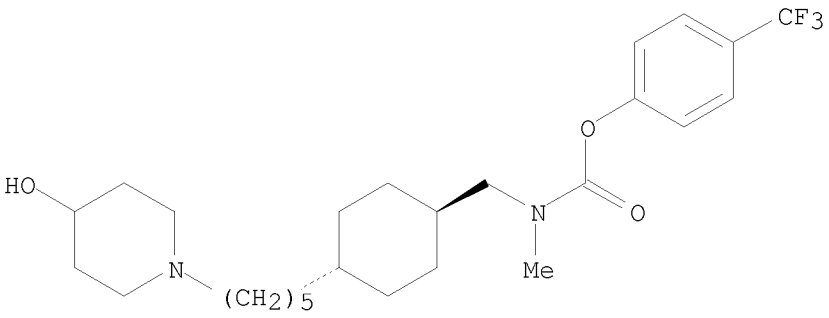


IT 554454-08-9P 554454-24-9P 554454-44-3P
554454-59-0P 554454-73-8P 554454-93-2P
554455-21-9P 554455-22-0P 554456-19-8P
554456-39-2P 554456-43-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclohexane derivs. as inhibitors of 2,3-oxidosqualene-lanosterol cyclase)

RN 554454-08-9 CAPLUS

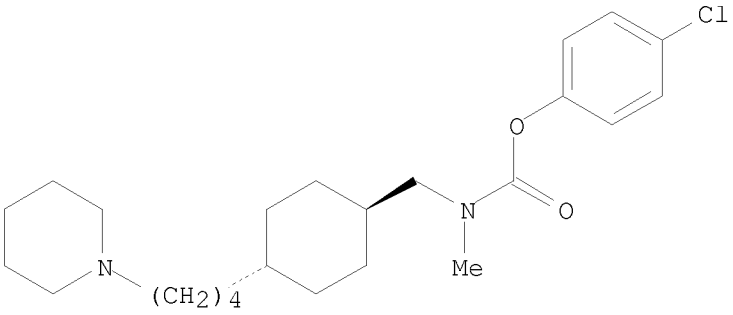
CN Carbamic acid, [[trans-4-[5-(4-hydroxy-1-piperidinyl)pentyl]cyclohexyl]methyl]methyl-, 4-(trifluoromethyl)phenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



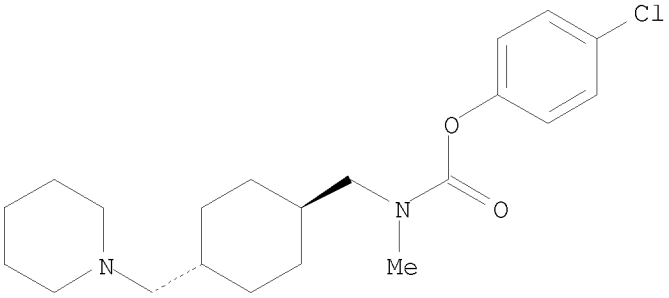
RN 554454-24-9 CAPLUS
CN Carbamic acid, methyl[[trans-4-[4-(1-piperidinyl)butyl]cyclohexyl]methyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 554454-44-3 CAPLUS
CN Carbamic acid, methyl[[trans-4-(1-piperidinylmethyl)cyclohexyl]methyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

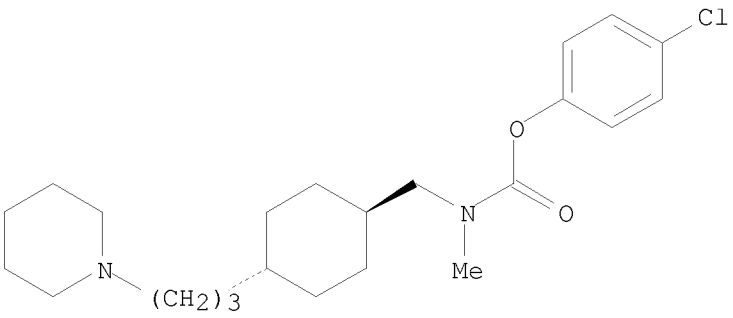
Relative stereochemistry.



RN 554454-59-0 CAPLUS
CN Carbamic acid, methyl[[trans-4-[3-(1-piperidinyl)propyl]cyclohexyl]methyl]-

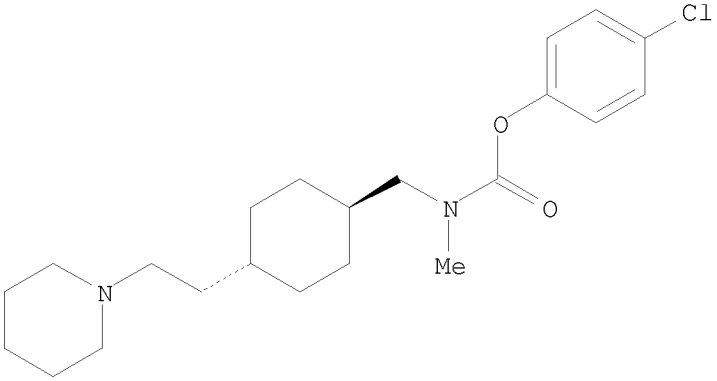
, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



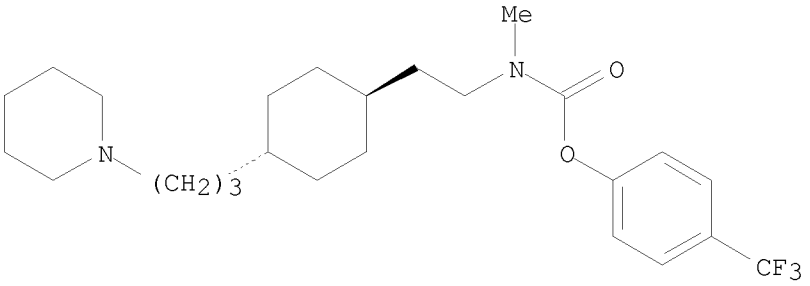
RN 554454-73-8 CAPLUS
CN Carbamic acid, methyl[[trans-4-[2-(1-piperidinyl)ethyl]cyclohexyl]methyl]-
, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



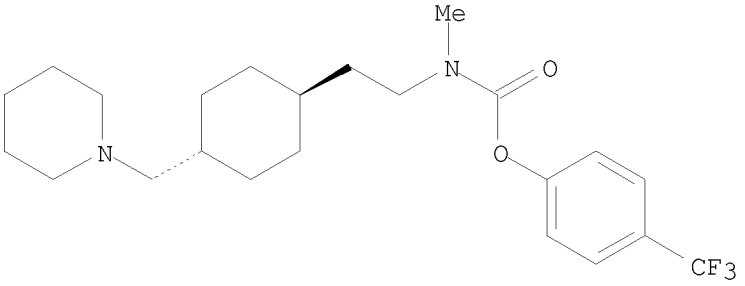
RN 554454-93-2 CAPLUS
CN Carbamic acid, methyl[2-[trans-4-[3-(1-
piperidinyl)propyl]cyclohexyl]ethyl]-, 4-(trifluoromethyl)phenyl ester
(9CI) (CA INDEX NAME)

Relative stereochemistry.



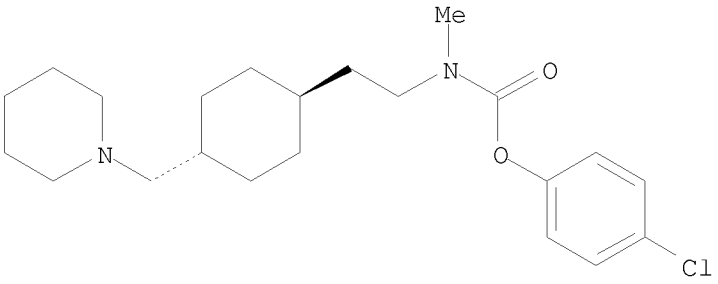
RN 554455-21-9 CAPLUS
CN Carbamic acid, methyl[2-[trans-4-(1-piperidinylmethyl)cyclohexyl]ethyl]-, 4-(trifluoromethyl)phenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



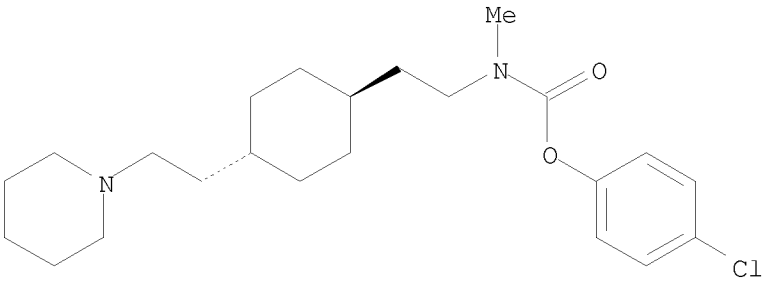
RN 554455-22-0 CAPLUS
CN Carbamic acid, methyl[2-[trans-4-(1-piperidinylmethyl)cyclohexyl]ethyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



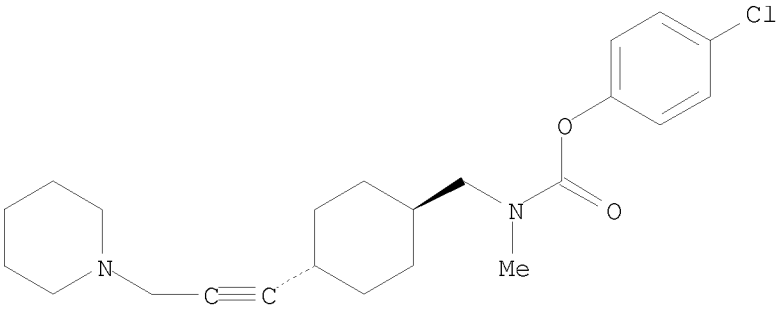
RN 554456-19-8 CAPLUS
CN Carbamic acid, methyl[2-[trans-4-[2-(1-piperidinyl)ethyl]cyclohexyl]ethyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



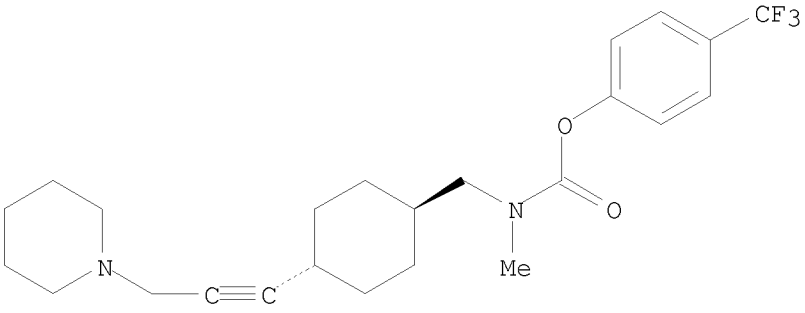
RN 554456-39-2 CAPLUS
CN Carbamic acid, methyl[[trans-4-[3-(1-piperidinyl)-1-propynyl]cyclohexyl]methyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 554456-43-8 CAPLUS
CN Carbamic acid, methyl[[trans-4-[3-(1-piperidinyl)-1-propynyl]cyclohexyl]methyl]-, 4-(trifluoromethyl)phenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:491050 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 139:63348
TITLE: Selective dopamine D3 receptor agonists for the treatment of sexual dysfunction
INVENTOR(S): Van der Graaf, Pieter Hadewijn; Wayman, Christopher Peter; Baxter, Andrew Douglas; Cook, Andrew Simon; Wong, Stephen Kwok-Fung
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 247 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2003051370	A1	20030626	WO 2002-GB5595		20021210	<--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW						
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
CA 2470624	A1	20030626	CA 2002-2470624		20021210	<--
AU 2002352372	A1	20030630	AU 2002-352372		20021210	<--
EP 1463508	A1	20041006	EP 2002-788092		20021210	<--
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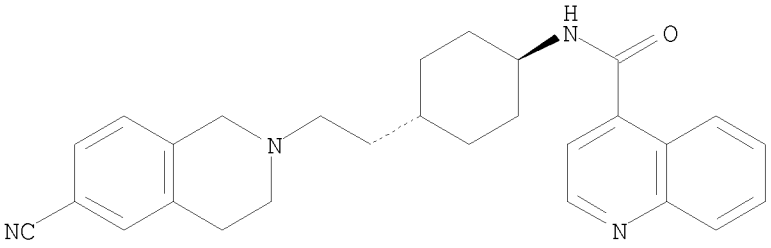
BR 2002015064	A	20041013	BR 2002-15064		20021210	<--
CN 1617727	A	20050518	CN 2002-825458		20021210	<--
JP 2005516014	T	20050602	JP 2003-552303		20021210	<--
NZ 533513	A	20060428	NZ 2002-533513		20021210	<--
ZA 2004003906	A	20050622	ZA 2004-3906		20040520	<--
MX 2004PA06079	A	20040927	MX 2004-PA6079		20040618	<--
US 20060052435	A1	20060309	US 2005-499210		20050826	<--
PRIORITY APPLN. INFO.:			GB 2001-30219	A	20011218	<--
			WO 2002-GB5595	W	20021210	<--

AB The use of a composition comprising a selective dopamine D3 receptor agonist is disclosed, wherein said dopamine D3 receptor agonist is at least about 15-times more functionally selective for a dopamine D3 receptor as compared with a dopamine D2 receptor when measured using the same functional assay, in the preparation of a medicament for the treatment and/or prevention of sexual dysfunction.

IT 215803-78-4, SB-277011
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(selective dopamine D3 receptor agonists for the treatment of sexual dysfunction)

RN 215803-78-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

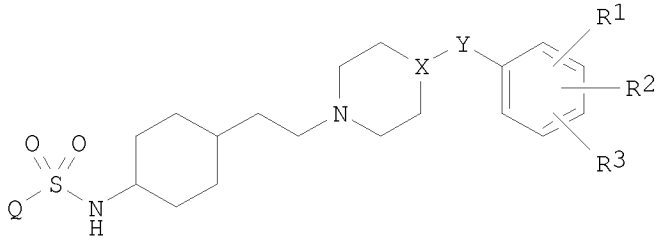
L18 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:282553 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 138:287701
TITLE: Preparation of N-[4-(2-heterocyclylethyl)cyclohexyl](hetero)arylsulfonamides as D3 receptor agonists for treatment of CNS and ophthalmic disorders
INVENTOR(S): Galambos, Janos; Nogradi, Katalin; Againe Csongor, Eva; Keseru, Gyoergy Miklos; Vago, Istvan; Domany, Gyoergy; Kiss, Bela; Gyertyan, Istvan; Laszlovszky, Istvan; Laszy, Judit
PATENT ASSIGNEE(S): Richter Gedeon Vegyeszeti Gyar Rt., Hung.
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003029233	A1	20030410	WO 2002-HU93	20020925 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
HU 2001003988	A2	20030528	HU 2001-3988	20010928 <--
HU 2001003988	A3	20050628		

AU 2002329500	A1	20030414	AU 2002-329500		20020925 <--
EP 1438302	A1	20040721	EP 2002-765129		20020925 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
JP 2005504126	T	20050210	JP 2003-532483		20020925 <--
US 20050107397	A1	20050519	US 2004-491150		20041022 <--
PRIORITY APPLN. INFO.:			HU 2001-3988	A	20010928 <--
			WO 2002-HU93	W	20020925 <--

OTHER SOURCE(S): MARPAT 138:287701

GI



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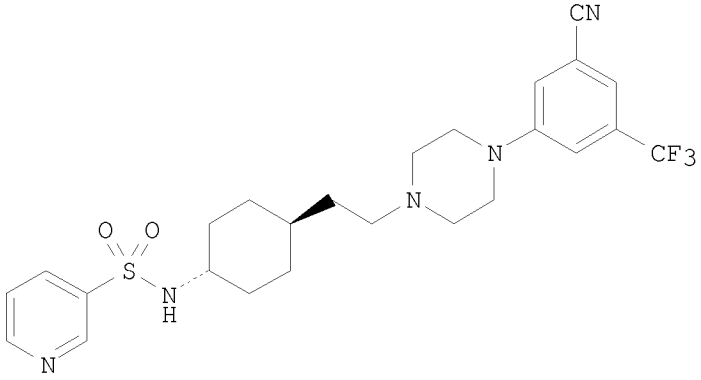


II

AB Title compds. I [wherein X = N or CH; when X = N, Y = a bond; or when X = CH, Y = O, NH, CH2, or OCH2; R1-R3 = independently H, halo, alkyl, alkoxy, CN, OH, CF3, alkylsulfonyloxy, CF3SO2O, alkanoyloxy, (alkyl)amino, alkanoylamino, alkylsulfonylamino, arylsulfonylamino, NH2CO, CO2H, (N-hydroxy)carbamimidoyl, hydroxycarbamoyl, thiocarbamoyl, sulfamoyl, or (un)substituted heterocyclyl or Ph; or 2 adjacent R1, R2, and R3 may combine to form an (un)substituted heterocyclyl group; Q = (un)substituted alkyl, aryl, aralkyl, or heteroaralkyl; and geometric isomers, stereoisomers, diastereomers, salts, hydrates, and solvates thereof] were prepared as D3 dopamine receptor subtype selective ligands. For example, reaction of 1-(3-cyano-5-trifluoromethylphenyl)piperazine with trans-2-[4-[(tert-butyloxycarbonyl)amino]cyclohexyl]acetaldehyde in the presence of sodium triacetoxyborohydride in CH2Cl2 gave the cyclohexylethylpiperazine (85.8%). Deprotection with HCl and EtOAc (98%), followed by sulfonylation with 3-pyridinesulfonyl chloride•HCl provided (trans)-II (54%). Sulfonamides I were also prepared on a solid support. Twelve compds. of the invention exhibited potent binding

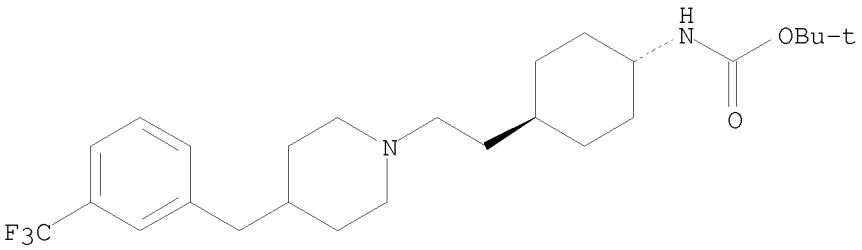
affinity at the D3 receptor with IC50 values ranging from 0.3 nM to 5.5 nM and showed 5 to 470 fold selectivity for the D3 over the D2 receptors. Thus, I are expected to be useful for the treatment of CNS and ophthalmic disorders related to D3 modulation while minimizing side effects associated with preferential blockade at the D2 receptor (no data).

IT 506427-92-5P, Trans-[4-[2-[4-(3-Trifluoromethylphenylmethyl)piperidin-1-yl]ethyl]cyclohexyl]carbamic acid tert-butyl ester 506427-93-6P, Trans-[4-[2-[4-(3-Fluorophenylmethyl)piperidin-1-yl]ethyl]cyclohexyl]carbamic acid tert-butyl ester 506427-94-7P, Trans-[4-[2-[4-(3-Cyanophenylmethyl)piperidin-1-yl]ethyl]cyclohexyl]carbamic acid tert-butyl ester 506427-96-9P, Trans-[4-[2-[4-(3-Trifluoromethylphenylamino)piperidin-1-yl]ethyl]cyclohexyl]carbamic acid tert-butyl ester 506427-97-0P, Trans-[4-[2-[4-(3-Trifluoromethylphenylmethoxy)piperidin-1-yl]ethyl]cyclohexyl]carbamic acid tert-butyl ester 506427-98-1P, Trans-[4-[2-[4-(3-Trifluoromethylphenoxy)piperidin-1-yl]ethyl]cyclohexyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of N-(heterocyclylethylcyclohexyl)(hetero)arylsulfonamides as D3 receptor agonists for treatment of CNS and ophthalmic disorders)

RN 506427-92-5 CAPLUS

CN Carbamic acid, [trans-4-[2-[4-[[3-(trifluoromethyl)phenyl]methyl]-1-piperidinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

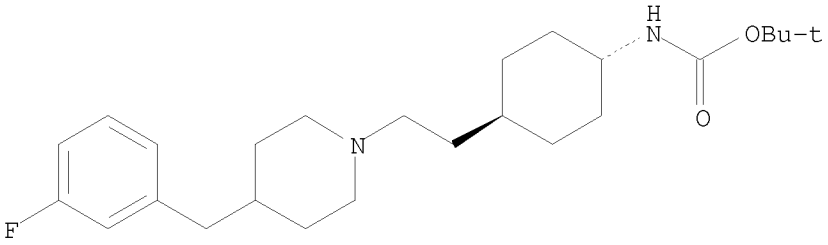
Relative stereochemistry.



RN 506427-93-6 CAPLUS

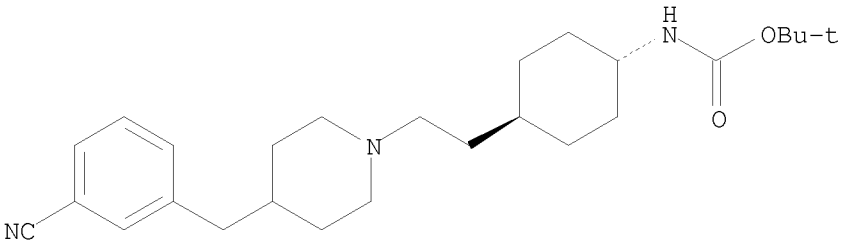
CN Carbamic acid, [trans-4-[2-[4-[(3-fluorophenyl)methyl]-1-piperidinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



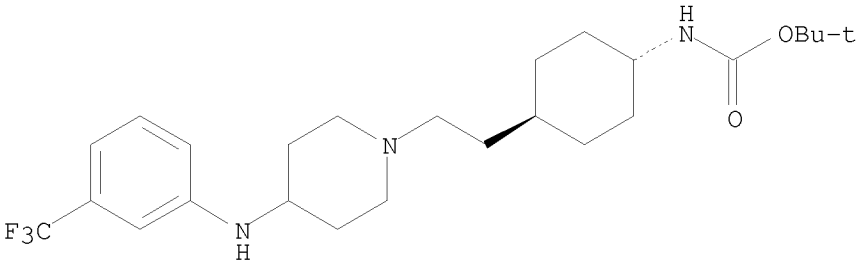
RN 506427-94-7 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[(3-cyanophenyl)methyl]-1-piperidinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



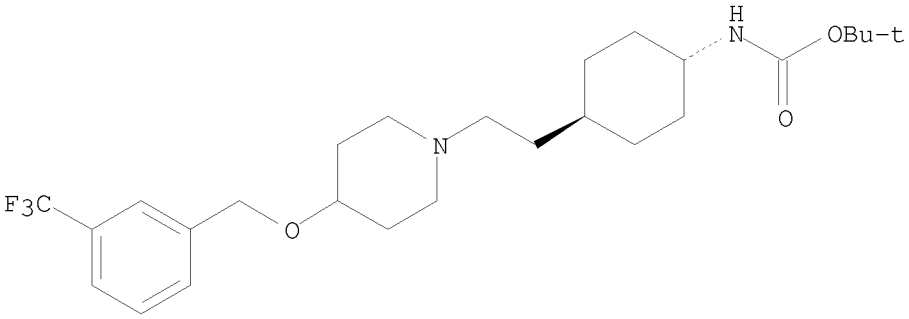
RN 506427-96-9 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[[3-(trifluoromethyl)phenyl]amino]-1-piperidinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



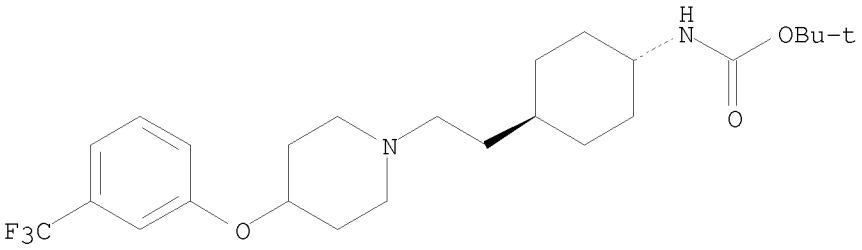
RN 506427-97-0 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[[3-(trifluoromethyl)phenyl]methoxy]-1-piperidinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 506427-98-1 CAPLUS
CN Carbamic acid, [trans-4-[2-[4-[3-(trifluoromethyl)phenoxy]-1-piperidinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:133024 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 138:163576
TITLE: Method for prevention or suppression of symptoms of psychosis
INVENTOR(S): Richtand, Neil
PATENT ASSIGNEE(S): The United States of America as Represented by Department of Veterans Affairs, USA
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003013507	A1	20030220	WO 2001-US24891	20010809 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001284761 A1 20030224 AU 2001-284761 20010809 <--
US 20040176467 A1 20040909 US 2004-486593 20040209 <--
PRIORITY APPLN. INFO.: WO 2001-US24891 W 20010809 <--

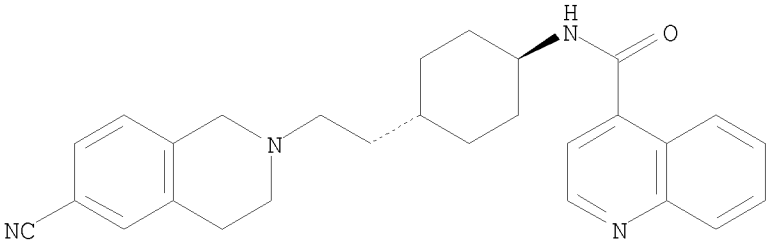
AB A method for prevention or suppression of symptoms of psychosis by treating non-psychotic patients who are at risk of developing psychosis is discosed. The method includes determining whether a patient is at risk for developing psychosis; making a diagnosis that the patient is at risk; and administering to the patient a selective D3 antagonist prior to the time the patient is psychotic in an amount sufficient to prevent or suppress symptoms of psychosis.

IT 215803-78-4, SB-277011
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(method for prevention or reducing occurrence of psychosis symptoms)

RN 215803-78-4 CAPLUS

CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:964330 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 138:39295
TITLE: Preparation of heterocyclic compounds as Rho-kinase inhibitors
INVENTOR(S): Imazaki, Naonori; Kitano, Masafumi; Ohashi, Naohito; Matsui, Kazuki
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Company, Limited, Japan
SOURCE: PCT Int. Appl., 425 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002100833	A1	20021219	WO 2002-JP5609	20020606 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002306284	A1	20021223	AU 2002-306284	20020606 <--
EP 1403255	A1	20040331	EP 2002-733352	20020606 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 20040138286	A1	20040715	US 2003-480526	20031212 <--
US 7199147	B2	20070403		

PRIORITY APPLN. INFO.:		JP 2001-176826	A	20010612 <--
		JP 2001-398992	A	20011228 <--
		WO 2002-JP5609	W	20020606 <--

OTHER SOURCE(S): MARPAT 138:39295

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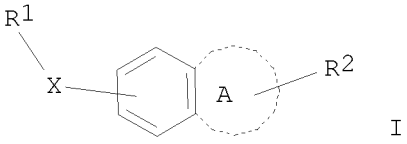


I

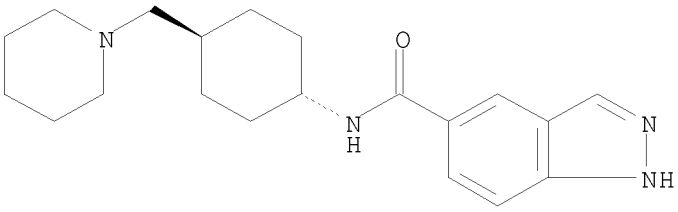
AB The title compds. I [wherein one to four groups represented by the general formula R1-X are present and may be the same or different from each other; A is a saturated or unsatd. five-membered heterocycle; X is a single bond, N(R3), O, S, or the like; R1 is hydrogen, halogeno, nitro, carboxyl, substituted or unsubstituted alkyl, or the like; R2 is hydrogen, halogeno, nitro, carboxyl, substituted or unsubstituted alkyl, or the like; and R3 is hydrogen, substituted or unsubstituted alkyl, or the like] are prepared N-(1-Benzyl-4-piperidinyl)-1H-indazole-5-amine dihydrochloride monohydrate in vitro showed IC50 of 0.4 μL/mL against Rho-kinase.

IT 478828-51-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. as Rho-kinase inhibitors)

RN 478828-51-2 CAPLUS

CN 1H-Indazole-5-carboxamide, N-[trans-4-(1-piperidinylmethyl)cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

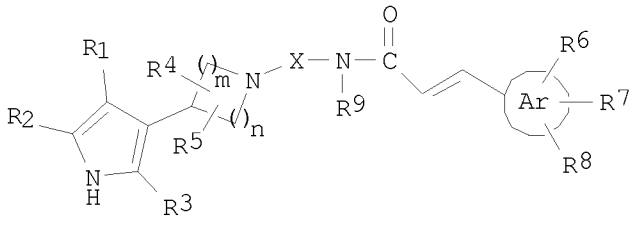


REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 11 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:777889 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 137:294868
TITLE: Preparation of 3-substituted indoles or fused pyrroles as antagonists of the chemokine MCP-1 (CCR2B) receptor
INVENTOR(S): Gribble, Andrew Derrick; Forbes, Ian Thomson; Witherington, Jason
PATENT ASSIGNEE(S): Smithkline Beecham P.L.C., UK
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002079151	A1	20021010	WO 2002-EP3570	20020328 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002253178	A1	20021015	AU 2002-253178	20020328 <--
PRIORITY APPLN. INFO.:			GB 2001-7904 A	20010329 <--
			GB 2001-7906 A	20010329 <--
			WO 2002-EP3570 W	20020328 <--

OTHER SOURCE(S): MARPAT 137:294868
GI



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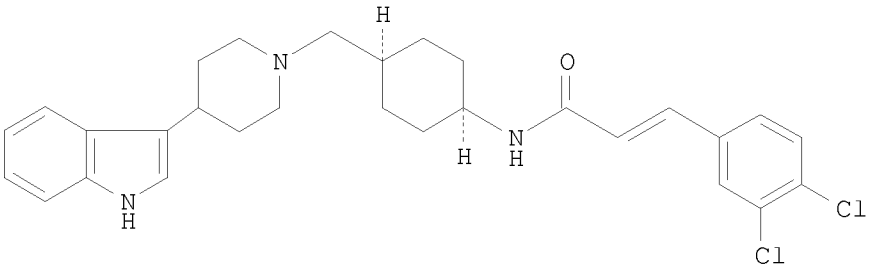


II

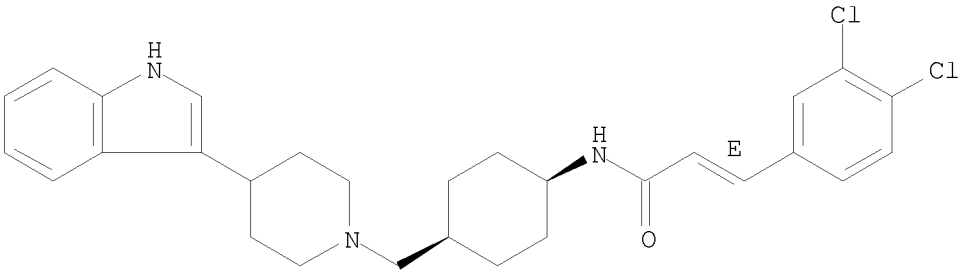
AB Title compds. I [Ar = (hetero)aryl group; R1-2 form the residue of a 5 to 7 membered monocyclic heteroaryl ring; R3 = H, alkyl; R4-5 = H, alkyl or together with the carbon atoms of the ring to which they are attached form a bridging 5-7-membered ring; R6-8 = H, halo, CN, alkyl, cycloalkyl, alkoxy, haloalkyl, hydroxy, amino, etc.; R9 = H, alkyl or arylalkyl; X = alkyl; m,n = 1-3] were prepared For instance, cis-4-tert-Butoxycarbonylamino-1-cyclohexanecarboxylic acid (preparation given) was reduced (THF, BH3•SMe2) and oxidized to the aldehyde (THF, DMSO, ClCOCOCl, TEA) and used to alkylate 4-(indol-3-yl)piperidine (CH2Cl2, NaHB(OAc)3). The resulting intermediate was deprotected (EtOH, HCl) and coupled to 3,4-dichlorocinnamic acid (CH2Cl2, EDCI, HOBt) to afford II. Selected example compds. had pKb in the range of 7.1 - 8.0 for the MCP-1 receptor. I are useful in treating inflammatory conditions with monocyte and/or lymphocyte involvement.

IT 374088-27-4P 374088-28-5P 374088-30-9P
374088-31-0P 467449-52-1P 467449-54-3P
467449-55-4P 467449-56-5P 467449-57-6P
467449-58-7P 467449-59-8P 467449-71-4P
468081-28-9P 468081-30-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(MCP-1 antagonist; 3-substituted indoles or fused pyrroles as antagonists of chemokine MCP-1 (CCR2B) receptor)

RN 374088-27-4 CAPLUS

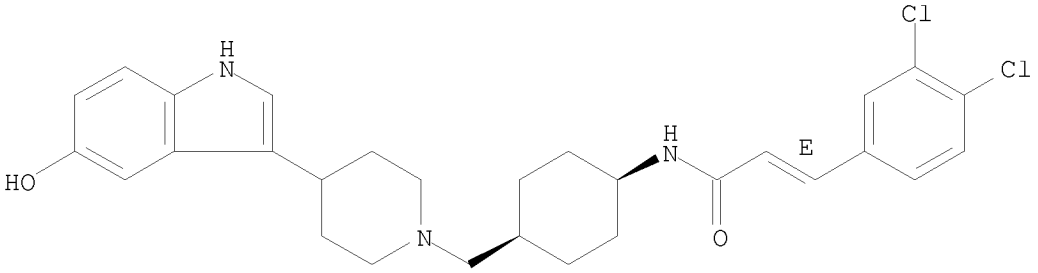
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



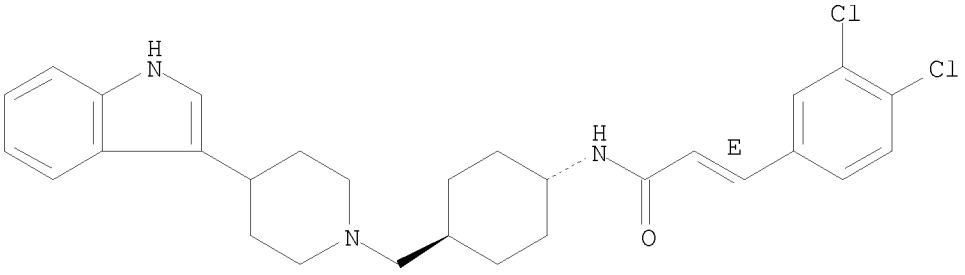
RN 374088-28-5 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(5-hydroxy-1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



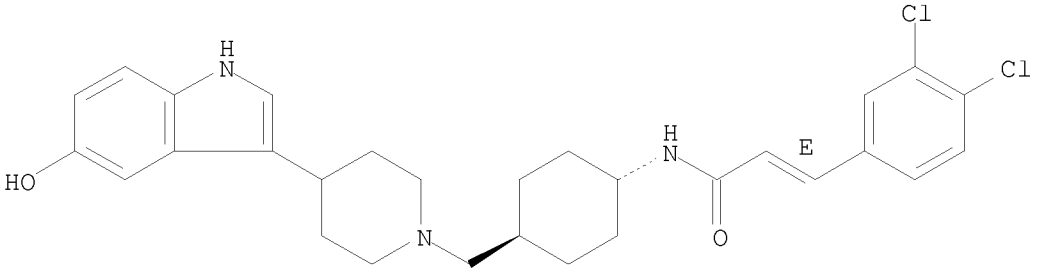
RN 374088-30-9 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[trans-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



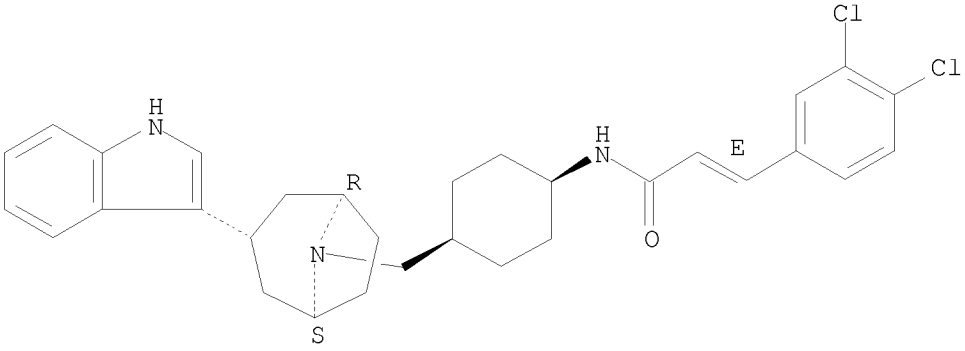
RN 374088-31-0 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[trans-4-[[4-(5-hydroxy-1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



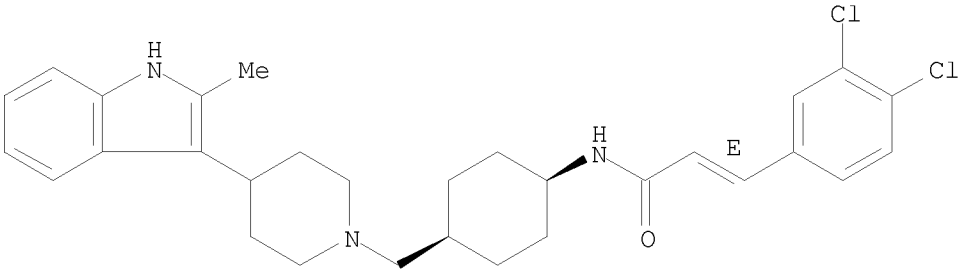
RN 467449-52-1 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[(3-exo)-3-(1H-indol-3-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



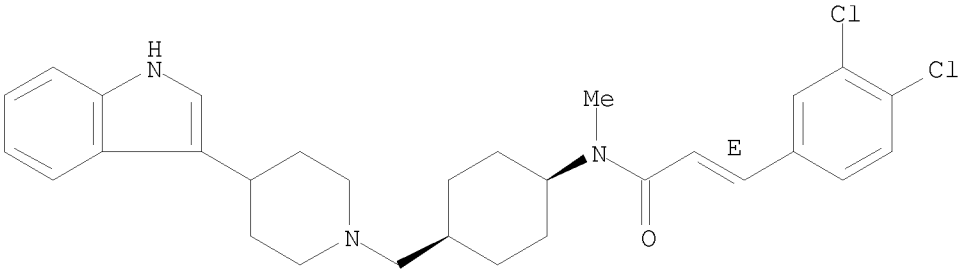
RN 467449-54-3 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(2-methyl-1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



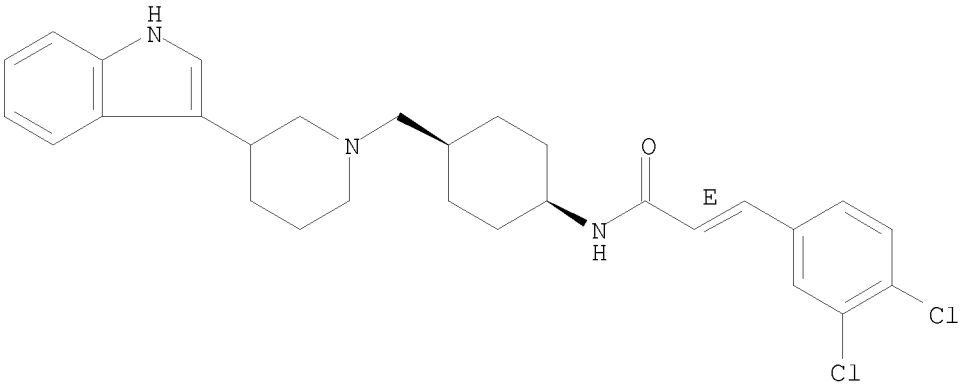
RN 467449-55-4 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-N-methyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



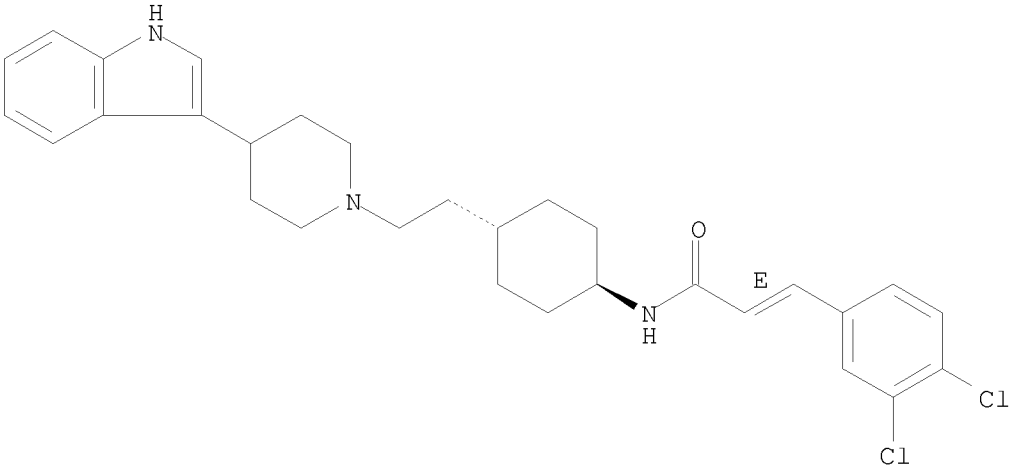
RN 467449-56-5 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[3-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



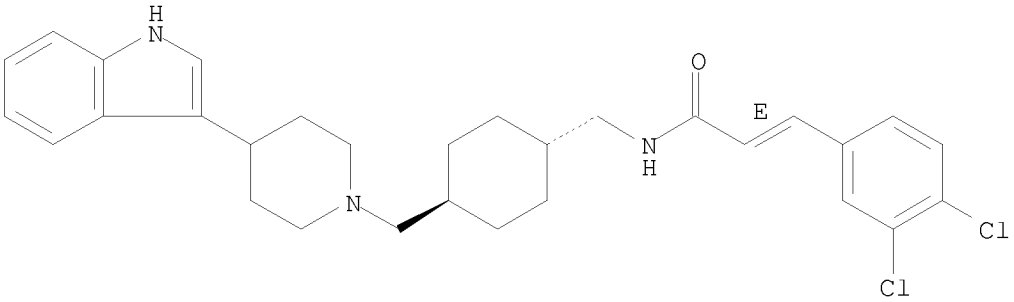
RN 467449-57-6 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[trans-4-[2-[4-(1H-indol-3-yl)-1-piperidinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



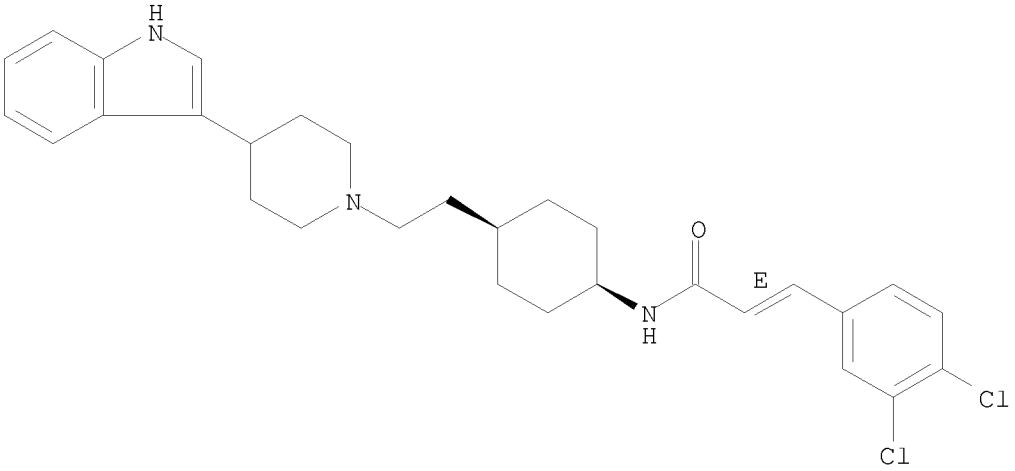
RN 467449-58-7 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[[trans-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]methyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



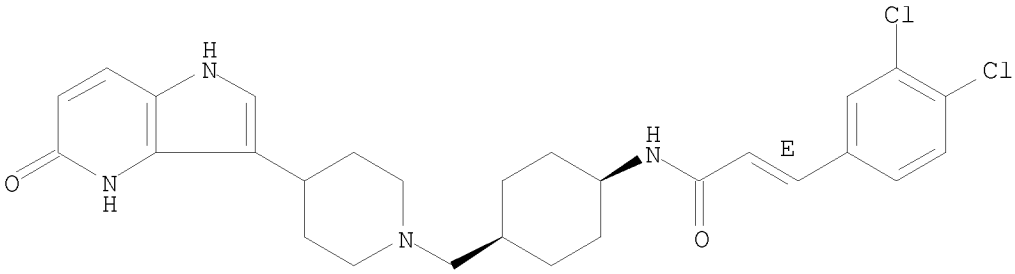
RN 467449-59-8 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[2-[4-(1H-indol-3-yl)-1-piperidinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



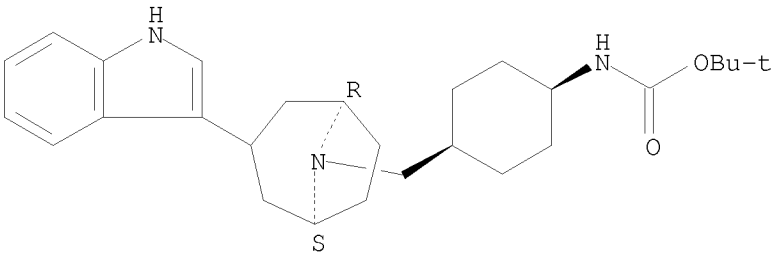
RN 467449-71-4 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(4,5-dihydro-5-oxo-1H-pyrrolo[3,2-b]pyridin-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



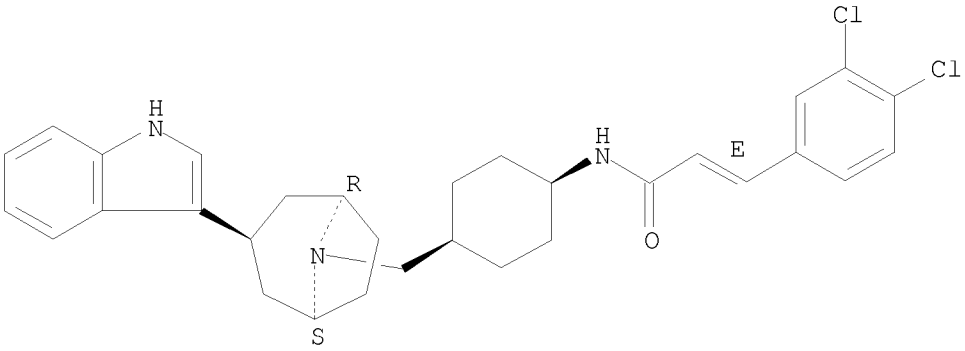
RN 468081-28-9 CAPLUS
CN Carbamic acid, [cis-4-[[(1R,5S)-3-(1H-indol-3-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



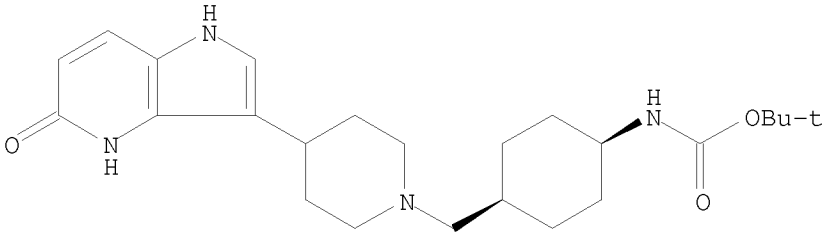
RN 468081-30-3 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[(3-endo)-3-(1H-indol-3-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



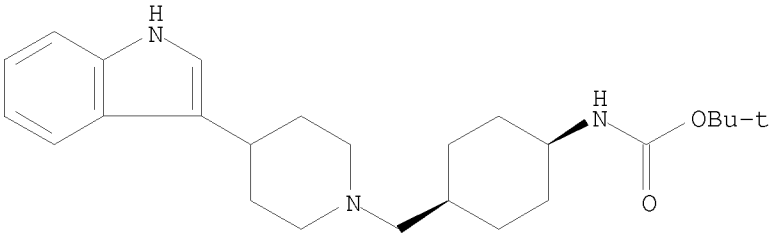
IT 467449-47-4P, cis-[4-[4-(5-Oxo-4,5-dihydro-1H-pyrrolo[3,2-b]pyridin-3-yl)piperidin-1-ylmethyl]cyclohexyl]carbamic acid tert-butyl ester 467449-49-6P, cis-1-((tert-Butoxycarbonyl)amino)-4-[[4-(1H-indol-3-yl)piperidin-1-yl]methyl]cyclohexane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; 3-substituted indoles or fused pyrroles as antagonists of chemokine MCP-1 (CCR2B) receptor)
RN 467449-47-4 CAPLUS
CN Carbamic acid, [cis-4-[[4-(4,5-dihydro-5-oxo-1H-pyrrolo[3,2-b]pyridin-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 467449-49-6 CAPLUS
CN Carbamic acid, [cis-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:142662 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 136:199955
TITLE: Preparation of aminocyclohexanes as OSC inhibitors for treatment of hypercholesterolemia, hyperlipemia, arteriosclerosis, and vascular diseases
INVENTOR(S): Ackermann, Jean; Aebi, Johannes; Blum, Denise; Chucholowski, Alexander; Dehmlow, Henrietta; Maerki, Hans-Peter; Morand, Olivier; Trussardi, Rene; Von der Mark, Elisabeth; Wallbaum, Sabine; Weller, Thomas
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 221 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002014267	A1	20020221	WO 2001-EP9174	20010808 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2418744	A1	20020221	CA 2001-2418744	20010808	<--
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EP 1311475	A1	20030521	EP 2001-974142	20010808	<--
EP 1311475	B1	20080806			
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JP 2004506037	T	20040226	JP 2002-519412	20010808	<--
HU 2003003105	A2	20040301	HU 2003-3105	20010808	<--
HU 2003003105	A3	20050530			
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US 20020045777	A1	20020418	US 2001-925188	20010809	<--
US 6858651	B2	20050222			
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IN 2003CN00218	A	20050408	IN 2003-CN218	20030204	<--
NO 2003000657	A	20030213	NO 2003-657	20030210	<--
MX 2003PA01269	A	20030609	MX 2003-PA1269	20030211	<--
US 20050176766	A1	20050811	US 2004-14374	20041215	<--
US 7335687	B2	20080226			

PRIORITY APPLN. INFO.:			EP 2000-117611	A 20000816	<--
			EP 2001-113646	A 20010619	<--
			WO 2001-EP9174	W 20010808	<--
			US 2001-925188	A3 20010809	<--

OTHER SOURCE(S): MARPAT 136:199955

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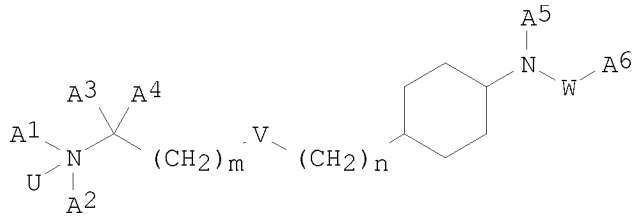

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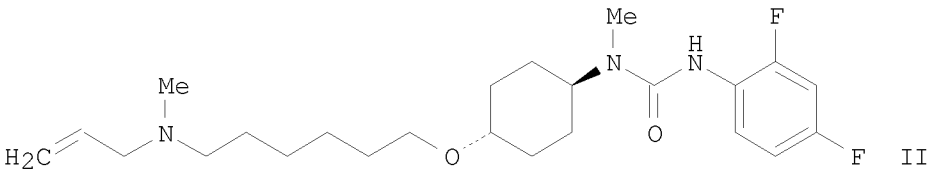


II

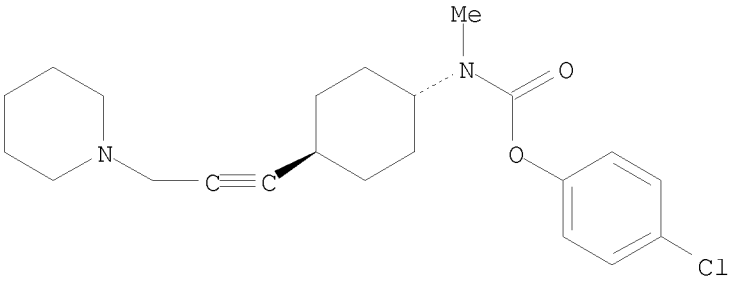
AB Title compds. I [wherein U = O or a lone pair; V = O, S, CH2, CH:CH, or C.tplbond.C; W = CO, CO2, CONR1, CSO, CSNR1, SO2, or SO2NR1; m and n = independently 0-7 and m + n = 0-7, with provisos; A1 = H, (hydroxy)alkyl, or alkenyl; A2 = (un)substituted alkyl, cycloalkyl(alkyl), or alkenyl; A3 and A4 = independently H or alkyl; or A1 and A2 or A1 and A3 or A3 and A4 may form a ring; A5 = H, (aryl)alkyl, or alkenyl; A6 = (cyclo)alkyl, aryl(alkyl), heteroaryl(alkyl), or alkoxycarbonylalkyl; R1 = H or alkyl; and pharmaceutically acceptable salts and/or esters thereof] were prepared Thus, trans-(4-hydroxycyclohexyl)methylcarbamic acid tert-Bu ester (preparation given) was etherified with 1,6-dibromohexane. Addition of N-allylmethylamine, followed by deprotection using TFA, afforded trans-[4-[4-(N-allylmethylamino)hexyloxy]cyclohexyl]methylamine. Coupling of the amine with 2,4-difluorophenylisocyanate in dioxane gave II. I are useful for the treatment and/or prophylaxis of diseases which are associated with 2,3-oxidosqualene-lanosterol cyclase (OSC), such as hypercholesterolemia, hyperlipemia, arteriosclerosis, vascular diseases, mycoses, gallstones, tumors and/or hyperproliferative disorders, and treatment and/or prophylaxis of impaired glucose tolerance and diabetes (no data).

IT 400896-64-2P 400896-68-6P 400896-97-1P
400897-27-0P 400897-30-5P 400897-91-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(OSC inhibitor; preparation of aminocyclohexanes as OSC inhibitors for treatment of hypercholesterolemia, hyperlipemia, arteriosclerosis, and vascular diseases)

RN 400896-64-2 CAPLUS

CN Carbamic acid, methyl[trans-4-[3-(1-piperidinyl)-1-propynyl]cyclohexyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

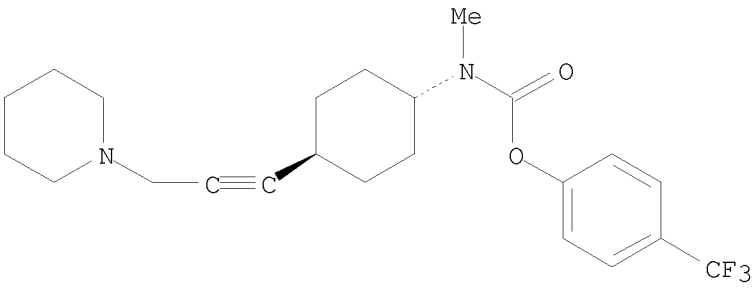
Relative stereochemistry.



RN 400896-68-6 CAPLUS

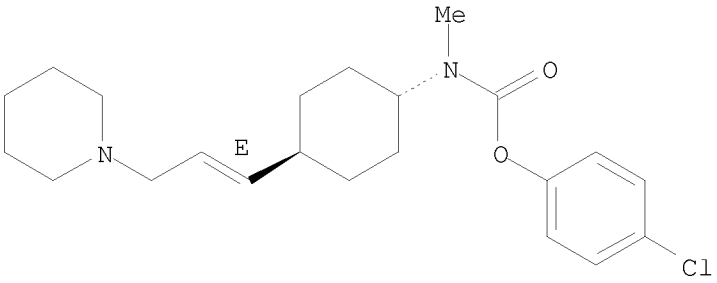
CN Carbamic acid, methyl[trans-4-[3-(1-piperidinyl)-1-propynyl]cyclohexyl]-, 4-(trifluoromethyl)phenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



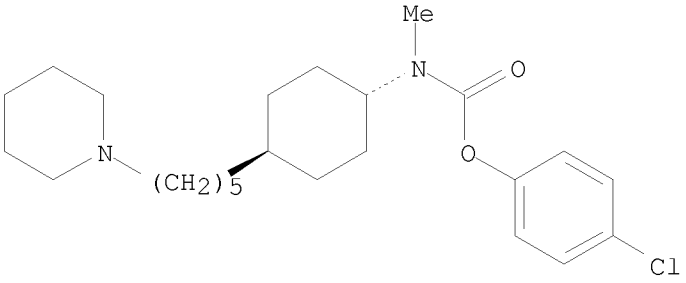
RN 400896-97-1 CAPLUS
CN Carbamic acid, methyl[trans-4-[(1E)-3-(1-piperidinyl)-1-propenyl]cyclohexyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



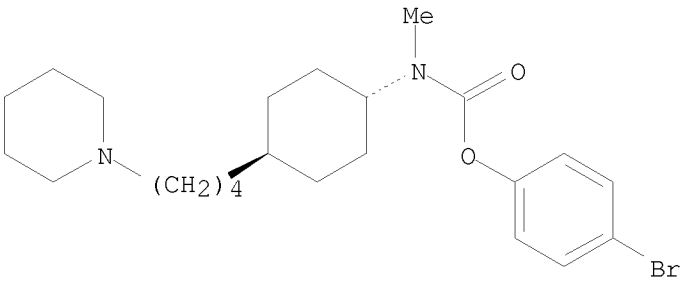
RN 400897-27-0 CAPLUS
CN Carbamic acid, methyl[trans-4-[5-(1-piperidinyl)pentyl]cyclohexyl]-, 4-chlorophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



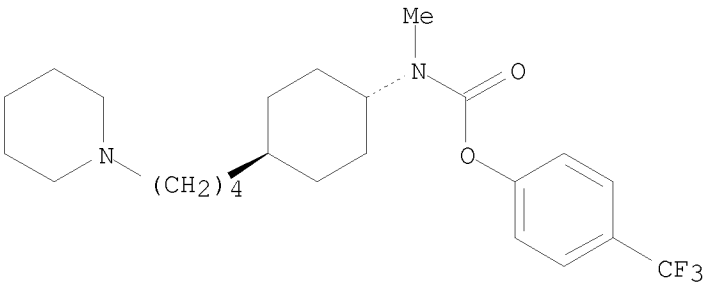
RN 400897-30-5 CAPLUS
CN Carbamic acid, methyl[trans-4-[4-(1-piperidinyl)butyl]cyclohexyl]-, 4-bromophenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 400897-91-8 CAPLUS
CN Carbamic acid, methyl[trans-4-[4-(1-piperidinyl)butyl]cyclohexyl]-, 4-(trifluoromethyl)phenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:113840 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 136:167283
TITLE: Preparation of acetylpiperidinebutanediamines as calcium ion-permeable AMPA receptor antagonists
INVENTOR(S): Mimura, Tetsuya; Kawajiri, Shinichi
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 93 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002047272	A	20020212	JP 2000-225300	20000726 <--
PRIORITY APPLN. INFO.:			JP 2000-225300	20000726 <--

OTHER SOURCE(S): MARPAT 136:167283

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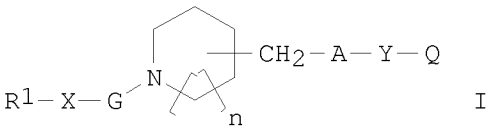


I

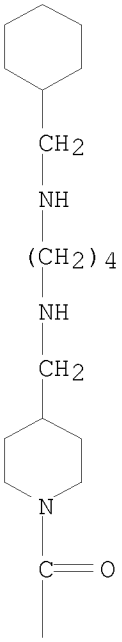
AB The compds. I (R1 = aryl, arylcarbonyl, aryloxy, cycloalkyl heterocyclyl, etc.; X = single bond, (un)substituted alkyl, alkenyl, cycloalkyl, monocyclic heterocyclyl; G = CO, SO2; n = 0-3; A = NR2, O, S, single bond; R2 = H, alkyl, OH; Y = alkylene, alkynylene, alkenylene; Q = NR3R4, OR5, SR5; R3, R4 = H, alkyl, cycloalkyl, aralkyl, etc.; R5 = alkyl, cycloalkyl, aryl, heterocyclyl, etc.), their salts, and solvates are prepared The compds. are useful for cerebral infarction, senile dementia, Alzheimer's, disease, Parkinson's disease, and Huntington's disease. Cyclohexanol was reacted with with oxalyl chloride in the presence of DMSO and Et3N in CH2Cl2 at -78° for 30 min and reacted with 4-[N-(4-aminobutyl)-N-(tert-butoxycarbonyl)aminomethyl]-1-(1-naphthylacetyl)piperidine for 1 h to give 82% N-(tert-butoxycarbonyl)-N'-cyclohexylmethyl-N-[1-(1-naphthylacetyl)piperidin-4-ylmethyl]-1,4-butanediamine, which was treated with HCl in EtOH at room temperature for 5 h to give N-cyclohexylmethyl-N'-[1-(1-naphthylacetyl)piperidin-4-ylmethyl]-1,4-butanediamine hydrochloride showing good AMPA receptor blocking activity in vitro.

IT 396071-20-8P 396072-34-7P 396072-35-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acetylpiperidinebutanediamines as calcium ion-permeable AMPA receptor antagonists)

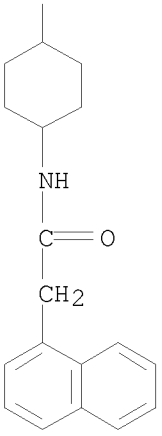
RN 396071-20-8 CAPLUS

CN 1-Naphthaleneacetamide, N-[4-[[4-[[[4-[(cyclohexylmethyl)amino]butyl]amino]methyl]-1-piperidinyl]carbonyl]cyclohexyl]-, hydrochloride (4:5) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

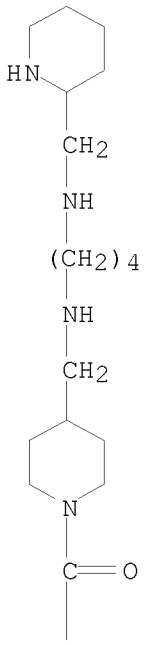


●5/4 HCl

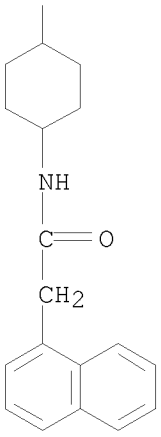
RN 396072-34-7 CAPLUS
CN 1-Naphthaleneacetamide, N-[4-[[4-[[[4-[(2-piperidinylmethyl)amino]butyl]amino]methyl]-1-

piperidinyl]carbonyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

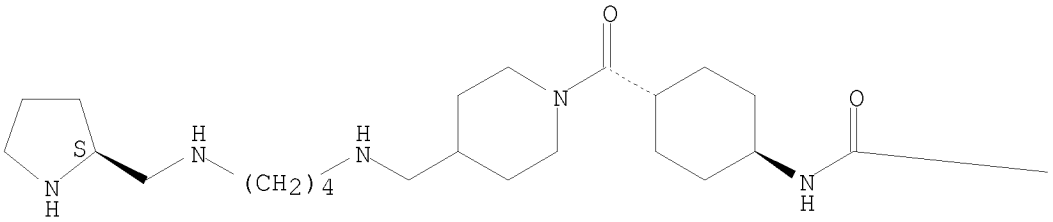


● HCl

RN 396072-35-8 CAPLUS
CN 1-Naphthaleneacetamide, N-[trans-4-[[4-[[[4-[[(2S)-2-pyrrolidinylmethyl]amino]butyl]amino]methyl]-1-piperidinyl]carbonyl]cyclohexyl]-, hydrochloride (1:3) (CA INDEX NAME)

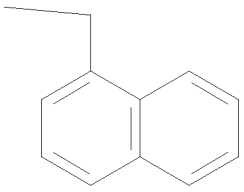
Absolute stereochemistry.

PAGE 1-A



●3 HCl

PAGE 1-B



L18 ANSWER 14 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:851115 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 136:5907
TITLE: Synthesis of aryl-amido-cyclohexane derivatives and their use as NK-1 receptor antagonists
INVENTOR(S): Castro Pineiro, Jose Luis; Dinnell, Kevin; Elliott, Jason Matthew; Hollingworth, Gregory John; Shaw,

Duncan Edward; Swain, Christopher John
PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK
SOURCE: PCT Int. Appl., 199 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001087838	A1	20011122	WO 2001-GB2145	20010516 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1286967	A1	20030305	EP 2001-929829	20010516 <--
EP 1286967	B1	20060927		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
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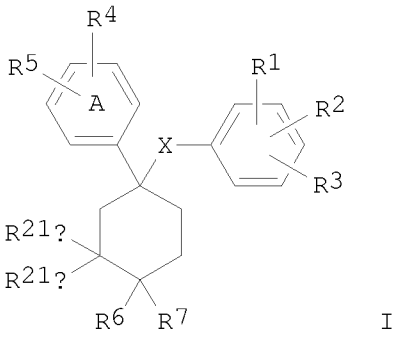
AU 2001256509	B2	20051222	AU 2001-256509	20010516 <--
AT 340781	T	20061015	AT 2001-929829	20010516 <--
ES 2273837	T3	20070516	ES 2001-929829	20010516 <--
US 20030236250	A1	20031225	US 2002-276127	20021113 <--
US 7105507	B2	20060912		

PRIORITY APPLN. INFO.: GB 2000-12240 A 20000519 <--
WO 2001-GB2145 W 20010516 <--
OTHER SOURCE(S): MARPAT 136:5907
GI



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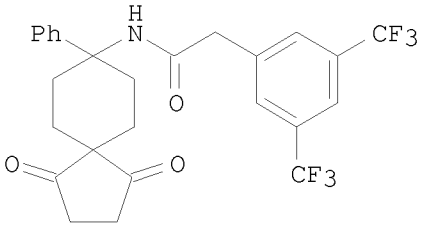


II

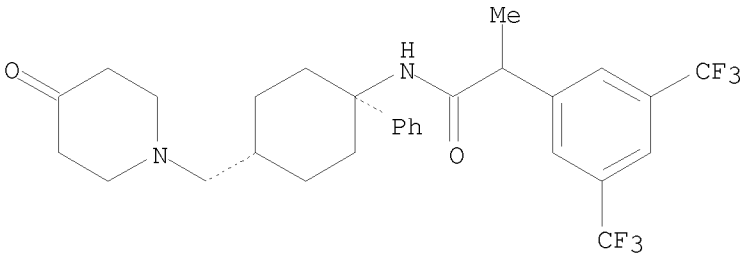
AB Title compds. I [ring A = Ph or pyridyl; X = linker selected from amido(carbonyl), amino, ester, ether; R1 = OH, (fluoro)alkyl, alkenyl, cycloalkyl, (fluoro)alkoxy, etc.; R2 = H, halo, alkyl, alkoxy or R1-2 with the atom to which they are attached, may form a 5 - 6 membered ring; R3 = H, halo, (fluoro)alkyl, (fluoro)alkoxy, cycloalkyl, CN, etc. or R3 = 5 - 6 membered heterocyclic ring; R4 = H, halo, (fluoro)alkyl, (fluoro)alkoxy, OH, NO2, CN, etc.; R5 = H, halo, (fluoro)alkyl, alkoxy; R6 = H, OH, alkyl; R7 = H, OH, alkylamino, alkylcarboxy, carbocyclyl, C-linked heterocyclyl or heteroaryl or R6-7 together represent :O, :CH-ester, ketal; R21a = H, halo, OH; R21b = H, or R21a-21b = F or together represent :O] were prepared Over 300 synthetic examples were disclosed. For instance, 3,5-bis(trifluoromethyl)benzeneacetic acid was converted to the acid chloride derivative (CH2Cl2, ClCOCOCl, DMF, room temperature, 1 h), and used to acylate 1,4-dioxo-8-phenylspiro[4.5]decan-8-amine (preparation given, dichloroethane, Et3N, room temperature) to give II as a brown gum in quant. yield. I are neurokinin 1 (NK-1) receptor antagonists (no data). Compds. I are of particular use in the treatment or prevention of depression, anxiety, pain, inflammation, migraine, emesis or postherpetic neuralgia.

IT 374793-74-5P 374793-94-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug; synthesis of aryl-amido-cyclohexane derivs. and use as NK-1 receptor antagonists)

RN 374793-74-5 CAPLUS

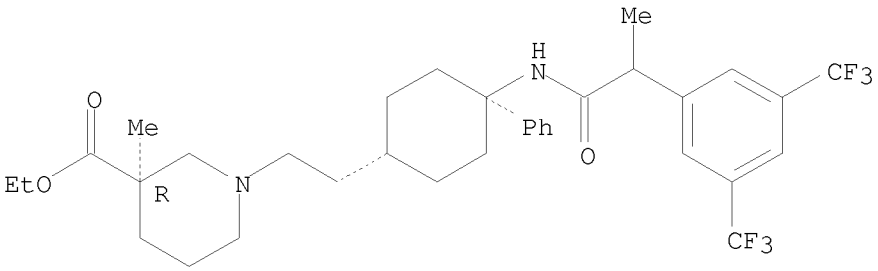
CN Benzeneacetamide, α-methyl-N-[trans-4-[(4-oxo-1-piperidinyl)methyl]-1-phenylcyclohexyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



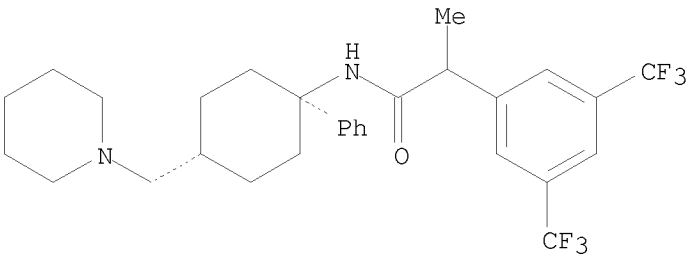
RN 374793-94-9 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[trans-4-[[2-[3,5-bis(trifluoromethyl)phenyl]-1-oxopropyl]amino]-4-phenylcyclohexyl]ethyl]-3-methyl-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



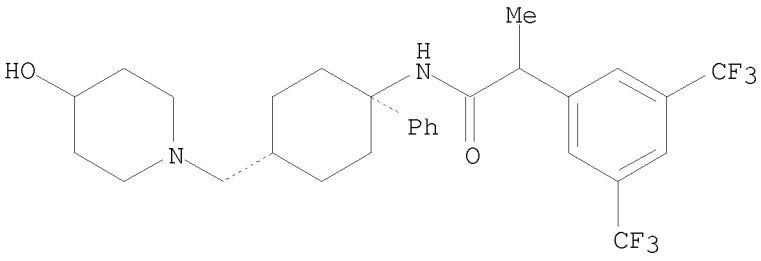
IT 374791-54-5P 374793-75-6P 374793-84-7P
374793-85-8P 374793-86-9P 374793-87-0P
374793-89-2P 374793-91-6P 374793-92-7P
374793-93-8P 374793-95-0P 374793-96-1P
374793-98-3P 374794-00-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; synthesis of aryl-amido-cyclohexane derivs. and use as NK-1 receptor antagonists)
RN 374791-54-5 CAPLUS
CN Benzeneacetamide, α-methyl-N-[trans-1-phenyl-4-(1-piperidinylmethyl)cyclohexyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



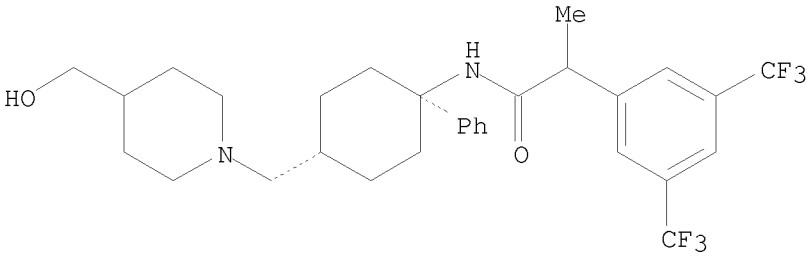
RN 374793-75-6 CAPLUS
CN Benzeneacetamide, N-[trans-4-[(4-hydroxy-1-piperidinyl)methyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



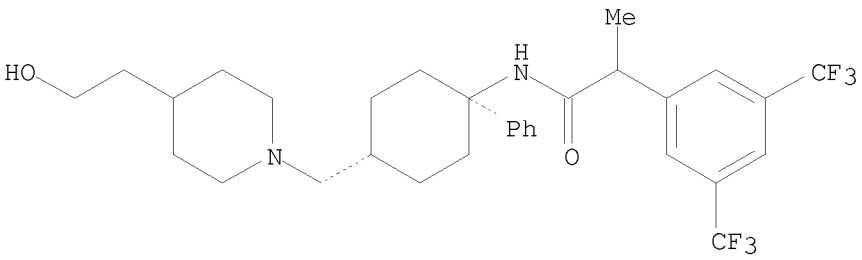
RN 374793-84-7 CAPLUS
CN Benzeneacetamide, N-[trans-4-[[4-(hydroxymethyl)-1-piperidinyl]methyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



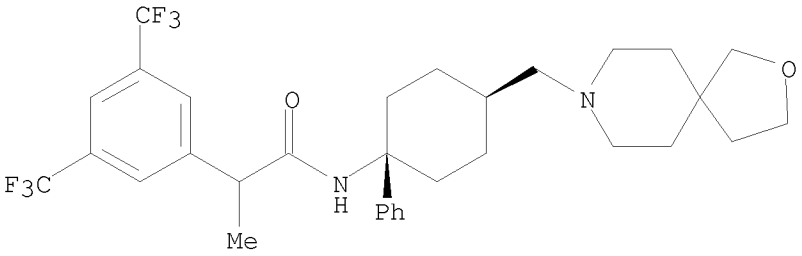
RN 374793-85-8 CAPLUS
CN Benzeneacetamide, N-[trans-4-[[4-(2-hydroxyethyl)-1-piperidinyl]methyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



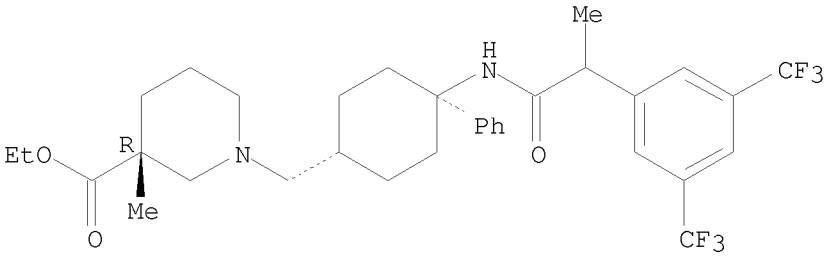
RN 374793-86-9 CAPLUS
CN Benzeneacetamide, α-methyl-N-[trans-4-(2-oxa-8-azaspiro[4.5]dec-8-ylmethyl)-1-phenylcyclohexyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



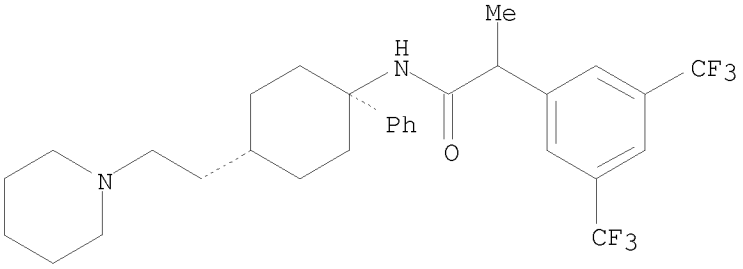
RN 374793-87-0 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[[trans-4-[[2-[3,5-bis(trifluoromethyl)phenyl]-1-oxopropyl]amino]-4-phenylcyclohexyl]methyl]-3-methyl-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



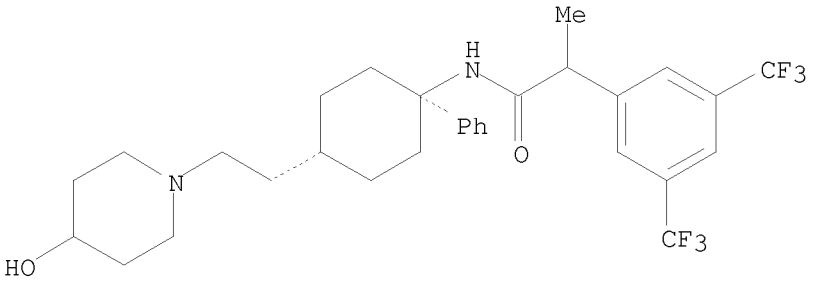
RN 374793-89-2 CAPLUS
CN Benzeneacetamide, α-methyl-N-[trans-1-phenyl-4-[2-(1-piperidinyl)ethyl]cyclohexyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



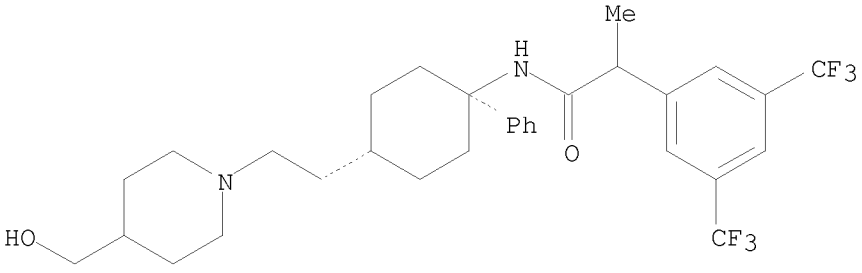
RN 374793-91-6 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(4-hydroxy-1-piperidinyl)ethyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



RN 374793-92-7 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-[4-(hydroxymethyl)-1-piperidinyl]ethyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

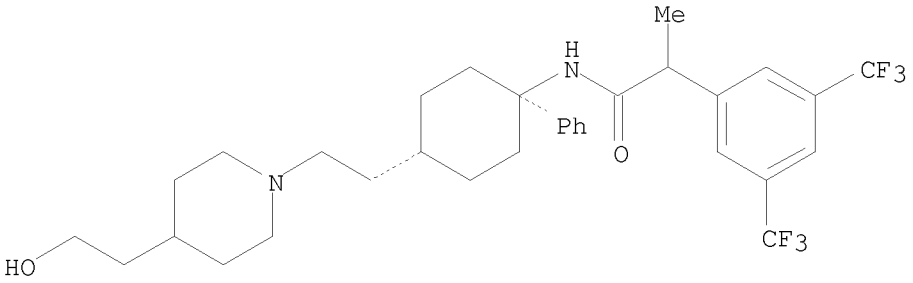
Relative stereochemistry.



RN 374793-93-8 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-[4-(2-hydroxyethyl)-1-piperidinyl]ethyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX

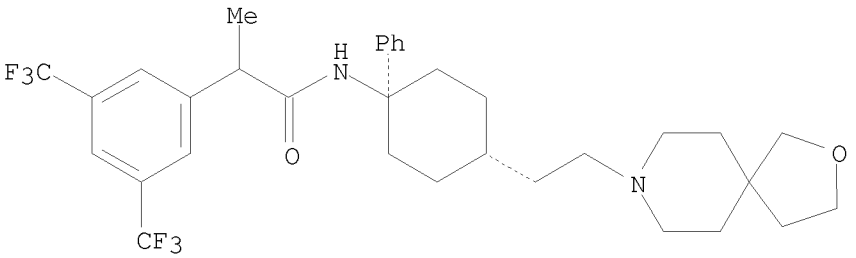
NAME)

Relative stereochemistry.



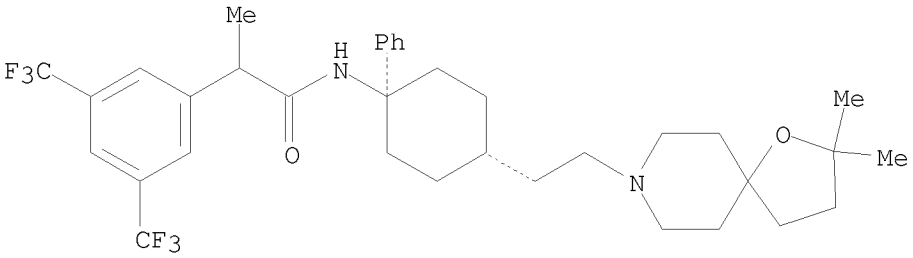
RN 374793-95-0 CAPLUS
CN Benzeneacetamide, α-methyl-N-[trans-4-[2-(2-oxa-8-azaspiro[4.5]dec-8-yl)ethyl]-1-phenylcyclohexyl]-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



RN 374793-96-1 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(2,2-dimethyl-1-oxa-8-azaspiro[4.5]dec-8-yl)ethyl]-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

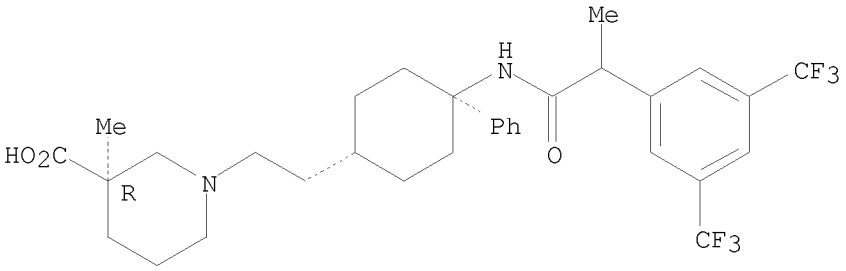
Relative stereochemistry.



RN 374793-98-3 CAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[trans-4-[[2-[3,5-

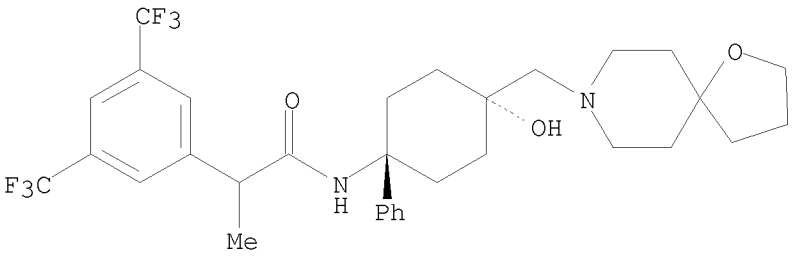
bis(trifluoromethyl)phenyl]-1-oxopropyl]amino]-4-phenylcyclohexyl]ethyl]-3-methyl-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 374794-00-0 CAPLUS
CN Benzeneacetamide, N-[cis-4-hydroxy-4-(1-oxa-8-azaspiro[4.5]dec-8-ylmethyl)-1-phenylcyclohexyl]-α-methyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:747751 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 135:303902
TITLE: Preparation of ethylenediamine and 1,2-cycloalkanediamine derivatives as inhibitors of activated blood coagulation factor X
INVENTOR(S): Yoshino, Toshiharu; Nagata, Tsutomu; Haginoya, Noriyasu; Yoshikawa, Kenji; Kanno, Hideyuki; Nagamochi, Masatoshi
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 481 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001074774	A1	20011011	WO 2001-JP2945		20010405 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
TW 288745	B	20071021	TW 2007-96119881		20010403 <--
TW 290136	B	20071121	TW 2001-90107988		20010403 <--
CA 2405144	A1	20011011	CA 2001-2405144		20010405 <--
AU 2001046835	A	20011015	AU 2001-46835		20010405 <--
EP 1270557	A1	20030102	EP 2001-919784		20010405 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001010052	A	20050510	BR 2001-10052		20010405 <--
RU 2268259	C2	20060120	RU 2002-129354		20010405 <--
AU 2001246835	B2	20060831	AU 2001-246835		20010405 <--
CN 1293057	C	20070103	CN 2001-808618		20010405 <--
ZA 2002007331	A	20030912	ZA 2002-7331		20020912 <--
IN 2002MN01273	A	20050304	IN 2002-MN1273		20020917 <--
KR 769592	B1	20071023	KR 2002-713005		20020930 <--
NO 2002004766	A	20021128	NO 2002-4766		20021003 <--
NO 324003	B1	20070730			
MX 2002PA09805	A	20030327	MX 2002-PA9805		20021004 <--
US 20040122063	A1	20040624	US 2003-240725		20030730 <--
US 7192968	B2	20070320			
HK 1056876	A1	20070525	HK 2003-109029		20031211 <--
US 20060004009	A1	20060105	US 2005-217837		20050902 <--
PRIORITY APPLN. INFO.:			JP 2000-108047	A	20000405 <--
			WO 2001-JP2945	W	20010405 <--
			US 2003-240725	A3	20030730

OTHER SOURCE(S): MARPAT 135:303902

AB Compds. of the general formula (1): Q1-Q2-CO-N(R1)-Q3-N(R2)-T1-Q4 [R1, R2 = H, OH, alkyl, alkoxy; Q1 = (un)substituted and (un)saturated 5- to 6-membered cyclohydrocarbyl or heterocyclyl or bi- or tricyclic condensed heterocyclyl; Q2 = bond, linear or branched alkyl C1-6 alkylene, C2-6 alkenylene, or C2-6 alkynylene, N-alkyl-(un)substituted NH or NH(CH2)m, (un)substituted and (un)saturated divalent 5- to 6-membered cyclic hydrocarbon or heterocycle or bi- or tricyclic condensed heterocycle group; Q3 = CR5R6CR7R8 (wherein R5, R6, R7, R8 = H, HO, halo, haloalkyl, cyano, cyanoalkyl, acyl, acylalkyl, alkyl, alkenyl, alkynyl, alkoxy, alkoxyalkyl, hydroxyalkyl, CO2H, carboxyalkyl, etc.), Q (wherein Q5 = C1-8 alkylene or C2-8 alkenylene; R9 and R10 are substituted on the carbon atoms of the ring containing Q5 and represent H, OH, alkyl, alkenyl, alkynyl, halo, haloalkyl, cyano, cyanoalkyl, NH2, aminoalkyl, N-alkylaminoalkyl, etc.); Q4 = (un)substituted aryl, arylalkenyl, heteroaryl, or heteroarylalkenyl, (un)substituted and (un)saturated bi- or tricyclic condensed hydrocarbyl or condensed heterocyclyl; T1 = CO, SO2] are prepared Also claimed are drugs which contain these compds. and are efficacious for thrombosis and embolism. Thus, (±)-cis-N1 (or

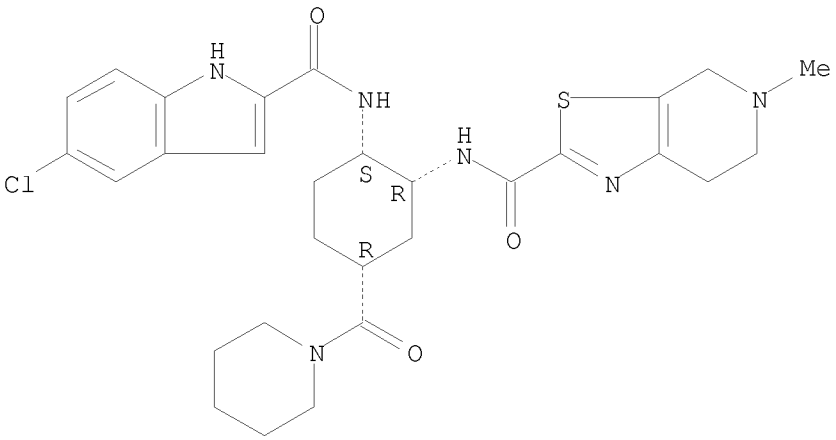
N2)-[(5-chloroindol-2-yl)carbonyl]-4,4-(1,2-ethylenedioxy)-1,2-cycloalkanediamine was condensed with 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine-2-carboxylic acid using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and 1-hydroxybenzotriazole monohydrate in DMF at room temperature overnight to give (±)-cis-N1 (or N2)-[(5-chloroindol-2-yl)carbonyl]-4,4-(1,2-ethylenedioxy)-N2 (or N1)-[(5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]-1,2-cyclohexanediamine (II). II in vitro showed IC50 of 1.4 nM μg/mL against human FXa.

IT 365995-49-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ethylenediamine and cycloalkanediamine derivs. as inhibitors of activated blood coagulation factor X for treatment of thrombosis and embolism)

RN 365995-49-9 CAPLUS

CN Thiazolo[5,4-c]pyridine-2-carboxamide, N-[(1R,2S,5R)-2-[[(5-chloro-1H-indol-2-yl)carbonyl]amino]-5-(1-piperidinylcarbonyl)cyclohexyl]-4,5,6,7-tetrahydro-5-methyl-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

REFERENCE COUNT: 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

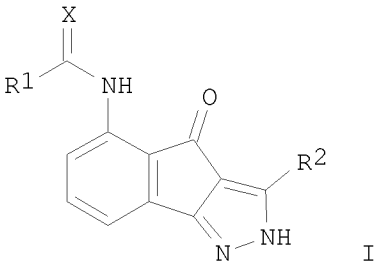
L18 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:731369 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 135:288778
TITLE: Preparation of indeno[1,2-c]pyrazol-4-ones as inhibitors of cyclin dependent kinases

INVENTOR(S): Nugiel, David A.; Carini, David J.; Dimeo, Susan V.; Yue, Eddy W.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA
SOURCE: U.S. Pat. Appl. Publ., 104 pp., Cont.-in-part of U.S. Ser. No. 639,618.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
US 20010027195	A1	20011004	US 2000-731304		20001206	<--
US 6407103	B2	20020618				
US 6413957	B1	20020702	US 2000-639618		20000815	<--
CA 2420164	A1	20020502	CA 2000-2420164		20001020	<--
AU 2001012168	A	20020506	AU 2001-12168		20001020	<--
EP 1414804	A1	20040506	EP 2000-973682		20001020	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY						
JP 2004524277	T	20040812	JP 2002-537713		20001020	<--

PRIORITY APPLN. INFO.:
US 1998-82476P P 19980421 <--
US 1999-295078 B1 19990420 <--
US 2000-639618 A2 20000815 <--
WO 2000-US28952 W 20001020 <--

OTHER SOURCE(S): MARPAT 135:288778
GI



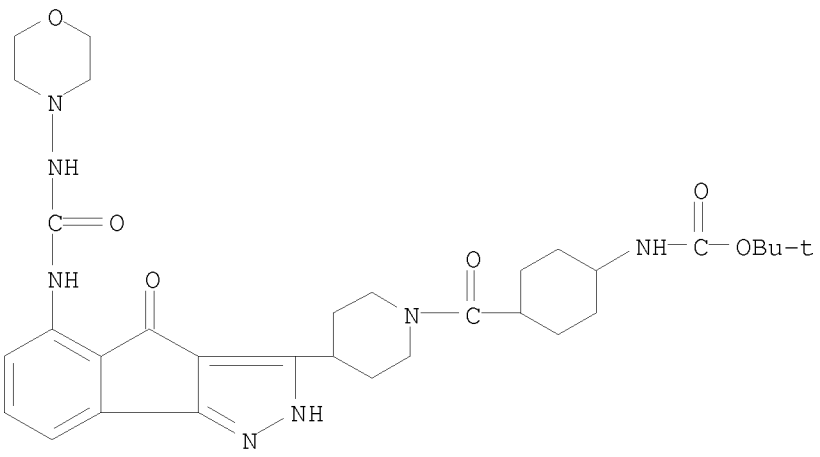
I

AB The present invention relates to the synthesis of a new class of indeno[1,2-c]pyrazol-4-ones of formula [X = O, S, (un)substituted NH; R1 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, NH2, C3-10 membered carbocyclyl, 3-10 membered heterocycle containing 1-4 heteroatoms selected from O, N, and S; R2 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, (CF2)mCF3, C3-10 membered carbocyclyl, 3-10 membered heterocycle containing 1-4 heteroatoms selected from O, N, and S; wherein m = 0, 1-4]. These compds. are potent inhibitors of the class of enzymes known as cyclin dependent kinases, which relate to the catalytic subunits cdk1-9 and their regulatory subunits know as cyclins A-H. This invention also provides a novel method of treating cancer or other proliferative diseases by administering a therapeutically effective amount of one of these compds. or a pharmaceutically acceptable salt form

thereof. Alternatively, cancer or other proliferative diseases can be treated by administering a therapeutically effective combination of one of the compds. of the present invention and one or more other known anti-cancer or anti-proliferative agents (no data). Thus, hydrogenation of di-Me 3-nitrophthalate over 5% Pd-C in methanol in a Parr shaker at 50 psi for 2 h followed by acetylation with Ac2O in pyridine at 25° for 2 h gave 79% di-Me 3-acetamidophthalate which was treated with NaH in DMF and cyclocondensed with 4-methoxyacetophenone at 90° for 20 min to give 30% 2-(4-methoxybenzoyl)-4-acetamidoindane-2,3-dione. Cyclocondensation of the latter triketone with hydrazine hydrate in the presence of p-TsOH in ethanol under reflux for 2 h gave I (R1 = Me, X = O, R2 = 4-methoxyphenyl).

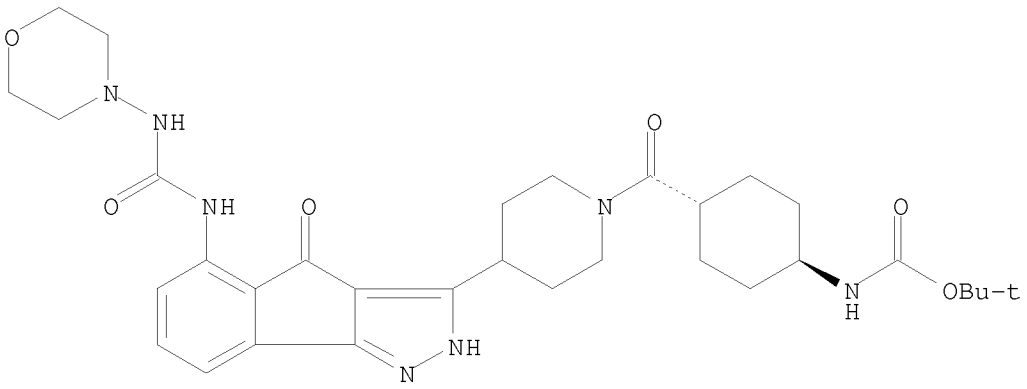
IT 364735-46-6P 364735-47-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indeno[c]pyrazolones as inhibitors of cyclin dependent kinases)

RN 364735-46-6 CAPLUS
CN Carbamic acid, [4-[[4-[2,4-dihydro-5-[[(4-morpholinylamino)carbonyl]amino]-4-oxoindeno[1,2-c]pyrazol-3-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 364735-47-7 CAPLUS
CN Carbamic acid, [trans-4-[[4-[2,4-dihydro-5-[[(4-morpholinylamino)carbonyl]amino]-4-oxoindeno[1,2-c]pyrazol-3-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:699660 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 136:31273
TITLE: Pharmacokinetics of the novel, high-affinity and selective dopamine D3 receptor antagonist SB-277011 in rat, dog, and monkey: in vitro/in vivo correlation and the role of aldehyde oxidase
AUTHOR(S): Austin, N. E.; Baldwin, S. J.; Cutler, L.; Deeks, N.; Kelly, P. J.; Nash, M.; Shardlow, C. E.; Stemp, G.; Thewlis, K.; Ayrton, A.; Jeffrey, P.
CORPORATE SOURCE: Department of Drug metabolism and Pharmacokinetics, GlaxoSmithKline, Welwyn, AL6 9AR, UK
SOURCE: Xenobiotica (2001), 31(8/9), 677-686
CODEN: XENOBH; ISSN: 0049-8254
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1. In vitro studies with the selective dopamine D3 receptor antagonist SB-277011 were conducted in liver microsomes and homogenates from rat, dog, cynomolgus monkey, and human to correlate the rate of metabolism with the in vivo pharmacokinetics of the compound in rat, dog, and cynomolgus monkey. 2. In the presence of NADPH, SB-277011 was relatively stable in the presence of liver microsomes from rat, dog, cynomolgus monkey, and human with an intrinsic clearance (CLi) of < 2 mL min-1 g-1 liver for all species. In total liver homogenates, SB-277011 was metabolized at a similar rate in rat and dog (CLi < 2 mL min-1 g-1 liver) to that in liver microsomes but in cynomolgus monkey and human (CLi = 9.9 and 45 mL min-1 g-1 liver, resp.) the intrinsic clearance was .apprx.6- and 35-fold higher, resp., than that in liver microsomes. 3. In the absence of NADPH, SB-277011 was rapidly cleared in liver homogenates from cynomolgus monkey and human (CLi = 7.4 and 27 mL min-1 g-1 liver, resp.) demonstrating that a significant pathway of metabolism of this compound was via an NADPH-independent non-microsomal oxidative route. This pathway was sensitive to inhibition with isovanillin suggesting that the enzyme responsible was aldehyde oxidase. 4. The in vivo pharmacokinetics showed that the plasma clearance of SB-277011 was low in rat (20 mL min-1 kg-1), moderate in dog (14 mL min-1 kg-1) and high in cynomolgus monkey (58 mL min-1 kg-1), which is consistent with the in vitro findings and

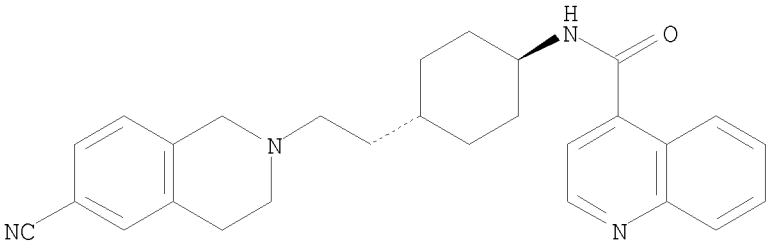
demonstrated a greater capacity for the monkey to metabolize this compound The oral bioavailability of SB-277011 in rat, dog, and cynomolgus monkey was 35, 43 and 2%, resp. Given the high clearance of this compound in cynomolgus monkey, the low oral bioavailability is probably as a result of high 1st-pass elimination, specifically by aldehyde oxidase, rather than poor absorption. 5. The high in vitro clearance of SB-277011 in human liver homogenates and the involvement of aldehyde oxidase in the metabolism of SB-277011 indicates that the bioavailability of the compound is likely to be low in human.

IT 215803-78-4, SB-277011
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacokinetics of dopamine D3 receptor antagonist SB-277011, in vitro/in vivo correlation)

RN 215803-78-4 CAPLUS

CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 18 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:612036 CAPLUS <<LOGINID::20081022>>

DOCUMENT NUMBER: 135:371606

TITLE: Conformationally restricted indolopiperidine derivatives as potent CCR2B receptor antagonists

AUTHOR(S): Witherington, J.; Bordas, V.; Cooper, D. G.; Forbes, I. T.; Gribble, A. D.; Ife, R. J.; Berkhout, T.; Gohil, J.; Groot, P. H. E.

CORPORATE SOURCE: Departments of Discovery Chemistry and Vascular Biology, GlaxoSmithKline Pharmaceuticals, Harlow, Essex, CM19 5AD, UK

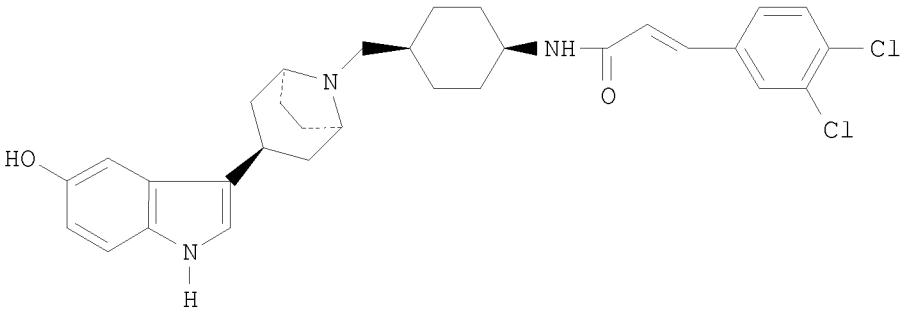
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(16), 2177-2180
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

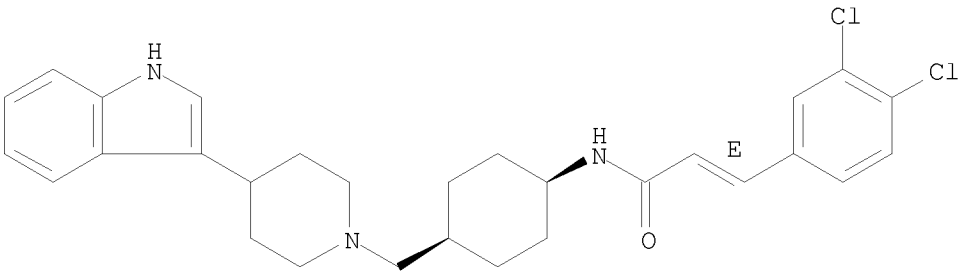
AB The preparation and biol. evaluation of a series of indolopiperidine CCR2B receptor antagonists possessing a conformationally restricted C-5 linker chain in combination with a restricted piperidine ring are described. Compared to the parent compound, the analog I shows a dramatic improvement in selectivity against a range of 5-HT and dopaminergic receptors.

IT 374088-27-4 374088-28-5 374088-30-9
374088-31-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(conformationally restricted indolopiperidine derivs. as potent CCR2B receptor antagonists)

RN 374088-27-4 CAPLUS

CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

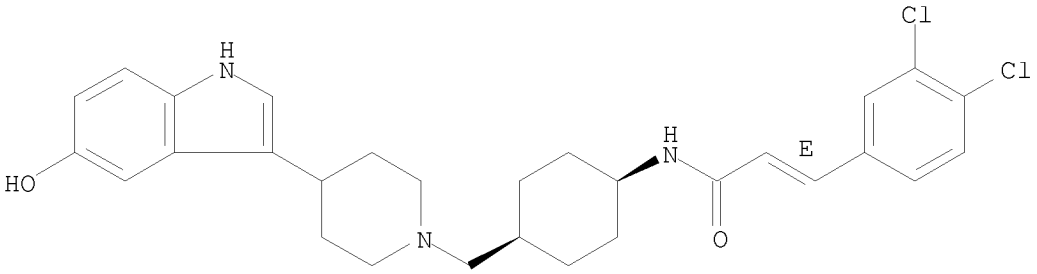
Relative stereochemistry.
Double bond geometry as shown.



RN 374088-28-5 CAPLUS

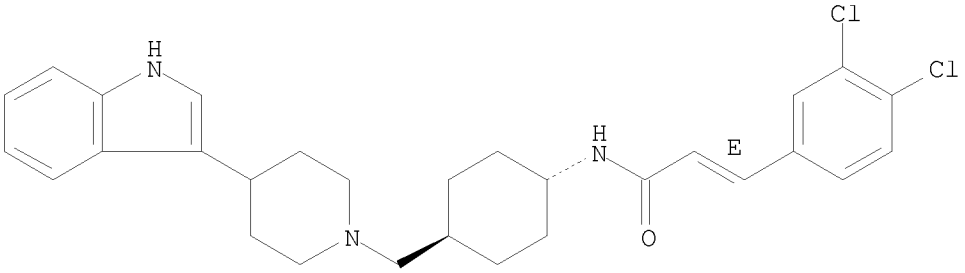
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[4-(5-hydroxy-1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



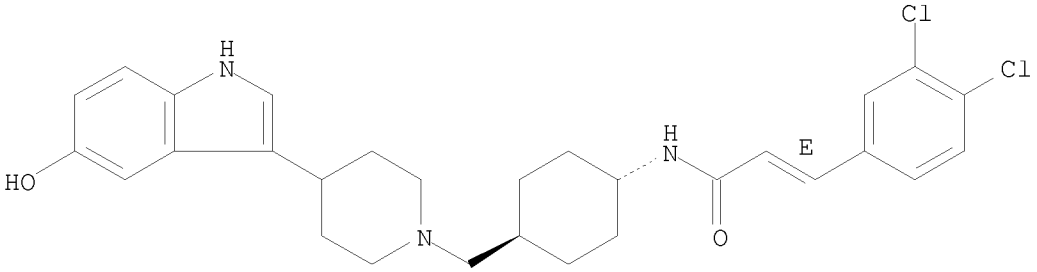
RN 374088-30-9 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[trans-4-[[4-(1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 374088-31-0 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[trans-4-[[4-(5-hydroxy-1H-indol-3-yl)-1-piperidinyl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

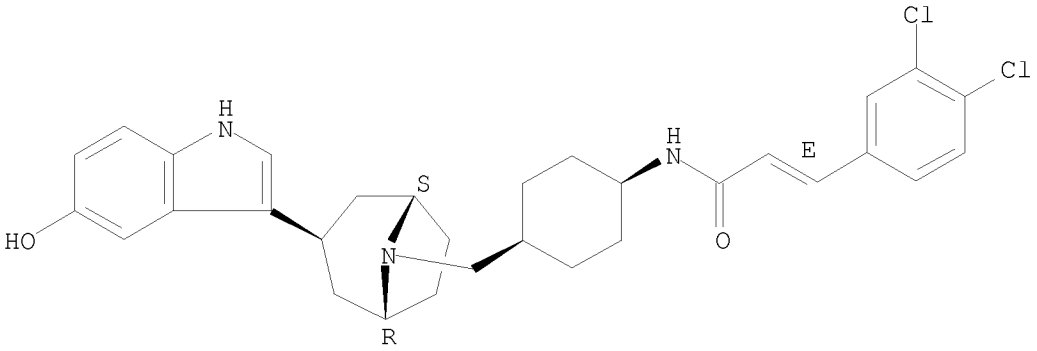
Relative stereochemistry.
Double bond geometry as shown.



IT 374088-24-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

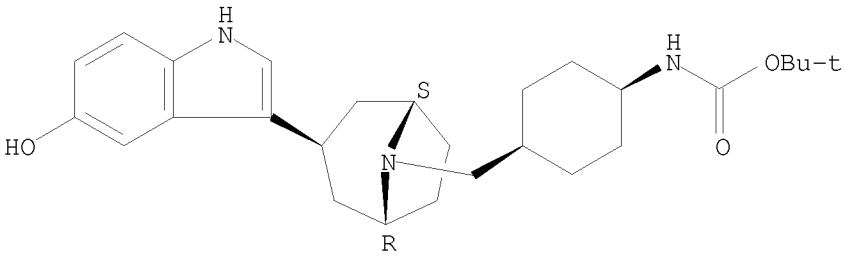
study); PREP (Preparation)
(conformationally restricted indolopiperidine derivs. as potent CCR2B receptor antagonists)
RN 374088-24-1 CAPLUS
CN 2-Propenamide, 3-(3,4-dichlorophenyl)-N-[cis-4-[[(3-exo)-3-(5-hydroxy-1H-indol-3-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



IT 374088-22-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(conformationally restricted indolopiperidine derivs. as potent CCR2B receptor antagonists)
RN 374088-22-9 CAPLUS
CN Carbamic acid, [cis-4-[[(3-exo)-3-(5-hydroxy-1H-indol-3-yl)-8-azabicyclo[3.2.1]oct-8-yl]methyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:607072 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 136:303360

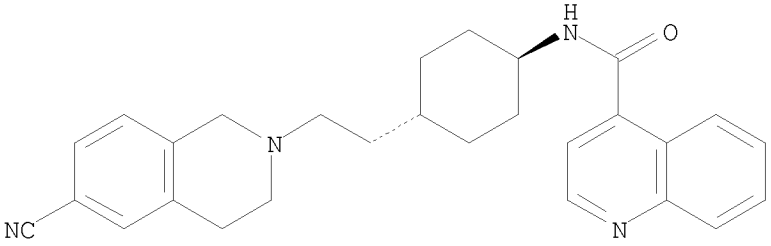
TITLE: SB-277011 (GlaxoSmithKline)
AUTHOR(S): Remington, Gary; Kapur, Shitij
CORPORATE SOURCE: Center for Addiction and Mental Health, Toronto, ON, M5T 1R8, Can.
SOURCE: Current Opinion in Investigational Drugs (PharmaPress Ltd.) (2001), 2(7), 946-949
CODEN: COIDAZ
PUBLISHER: PharmaPress Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. It is presumed that GlaxoSmithKline has taken over from SmithKline Beecham in investigating the highly selective dopamine D3 antagonist SB-277011 and its analogs for the potential treatment of schizophrenia, following the merger of Glaxo Wellcome and SmithKline Beecham in Dec. 2000. In June 2000, it was reported that novel 2,3,4,5-tetrahydro-1H-benzazepines and 2,3-dihydro-1H-isoindoles, including SB-277011, had shown high affinity and selectivity for the dopamine D3 receptor. All the compds. were suggested to have further potential roles in the treatment of drug abuse and psychosis. In Nov. 2000, data presented at the 30th Neuroscience meeting in New Orleans, LA, demonstrated that D3 receptor blockade with SB-277011 specifically altered neurochem. effects in the nucleus accumbens without the nonselective effects, such as catalepsy, seen with some other antagonists.

IT 215803-78-4P, SB 277011
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pharmacol. of dopamine D3 antagonist SB-277011)

RN 215803-78-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 20 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:241752 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 134:266206
TITLE: Preparation of 11-piperidinylbenzo[5,6]cyclohepta[1,2-b]pyridines and related compounds as inhibitors of farnesyl protein

transferase.

INVENTOR(S): Remiszewski, Stacy W.; Doll, Ronald J.; Alvarez, Carmen; Lalwani, Tarik

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: U.S., 57 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6211193	B1	20010403	US 1998-94720	19980615 <--
US 20010007870	A1	20010712	US 2001-768918	20010124 <--
US 6410541	B2	20020625		

PRIORITY APPLN. INFO.: US 1997-49953P P 19970617 <--
US 1998-94720 A3 19980615 <--

OTHER SOURCE(S): MARPAT 134:266206

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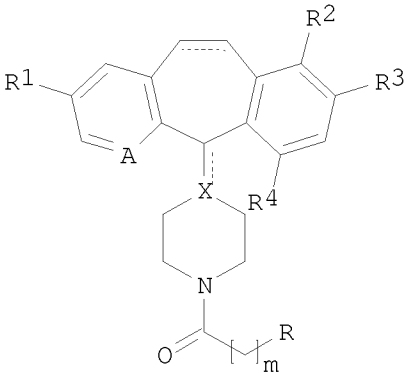

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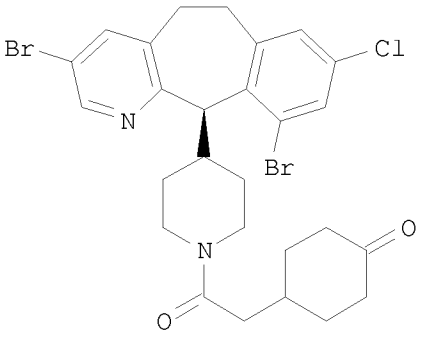


II

AB The title compds. [I; A = N, NO; R1, R3 = halo; R2, R4 = H, halo provided that ≥1 = H; X = C, CH, N; R = substituted cycloalkyl, heterocycloalkyl; dotted lines = optional double bonds; m = 0-2; R = substituted cyclobutyl(idene), cyclopentyl(idene), cyclohexyl(idene), indanyl(idene), azetidinyl, piperidinyl, etc.], were prepared Thus, tested I including title compound (II) inhibited farnesyl protein transferase with IC50's in the range 1.9 nM to 170 nM.

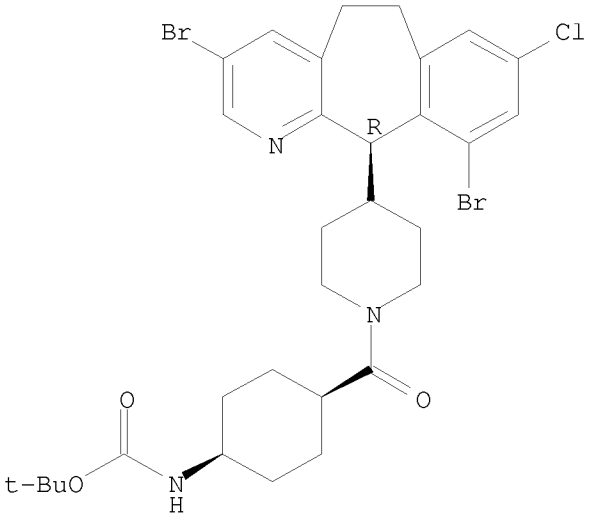
IT 218772-00-0P 218772-01-1P 218772-02-2P
218772-03-3P 218772-08-8P 218772-09-9P
218772-10-2P 218772-11-3P 218772-14-6P
218772-15-7P 218772-16-8P 218772-17-9P
218772-27-1P 218772-28-2P 218772-29-3P
218772-30-6P 218772-31-7P 218772-35-1P
218772-36-2P 218772-37-3P 218772-93-1P
218772-94-2P 218772-95-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 11-piperidinylbenzo[5,6]cyclohepta[1,2-b]pyridines and related compds. as inhibitors of farnesyl protein transferase)

RN 218772-00-0 CAPLUS

CN Carbamic acid, [cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

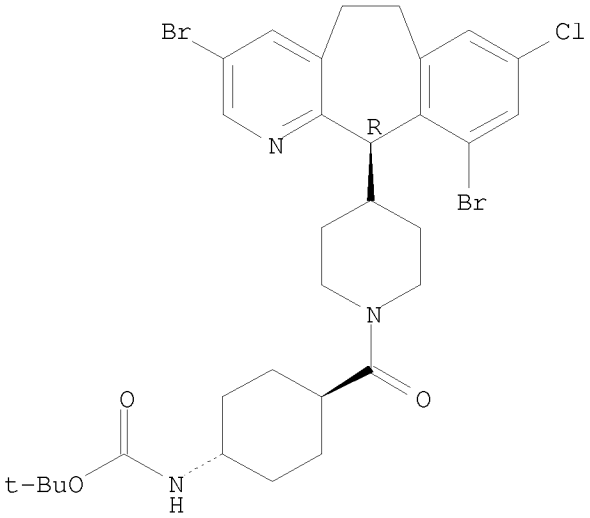
Absolute stereochemistry.



RN 218772-01-1 CAPLUS

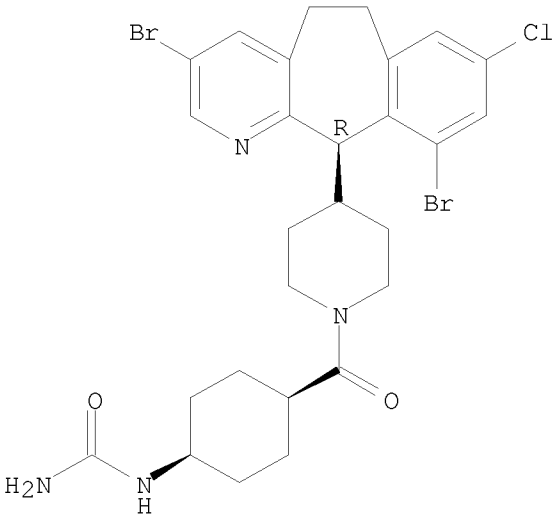
CN Carbamic acid, [trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



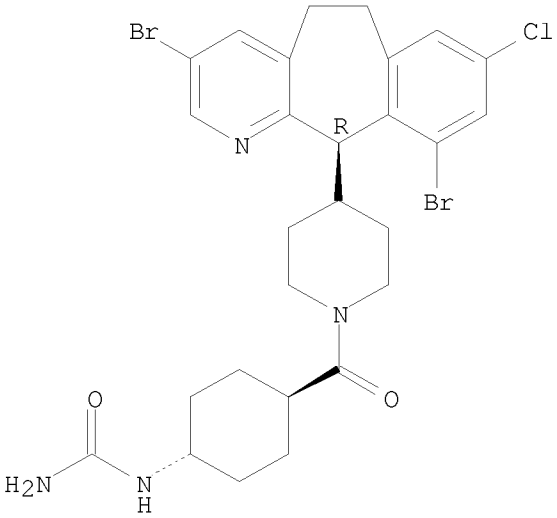
RN 218772-02-2 CAPLUS
CN Urea, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



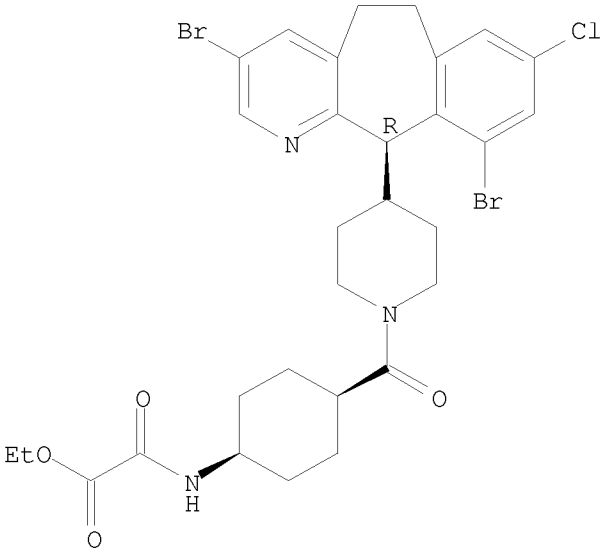
RN 218772-03-3 CAPLUS
CN Urea, N-[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



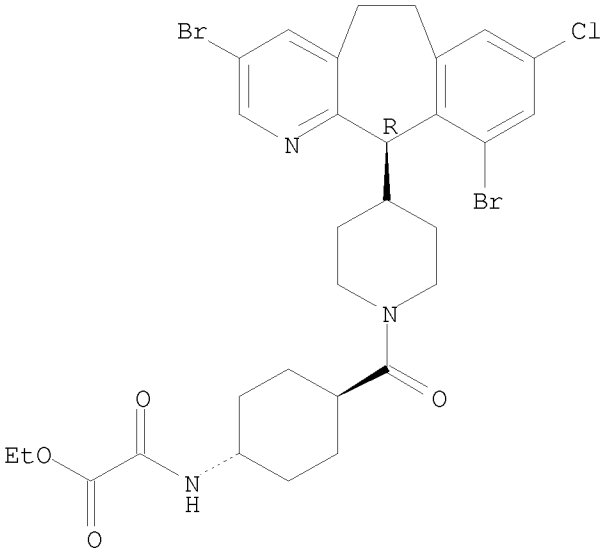
RN 218772-08-8 CAPLUS
CN Acetic acid, 2-[[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



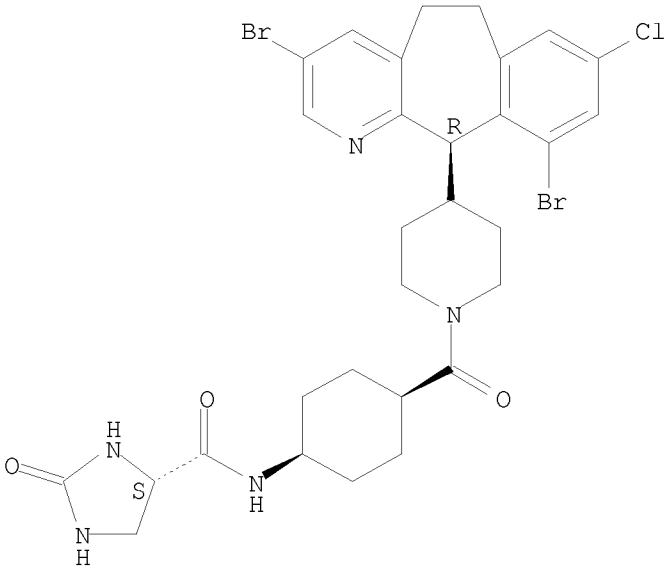
RN 218772-09-9 CAPLUS
CN Acetic acid, 2-[[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 218772-10-2 CAPLUS
CN 4-Imidazolidinecarboxamide, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

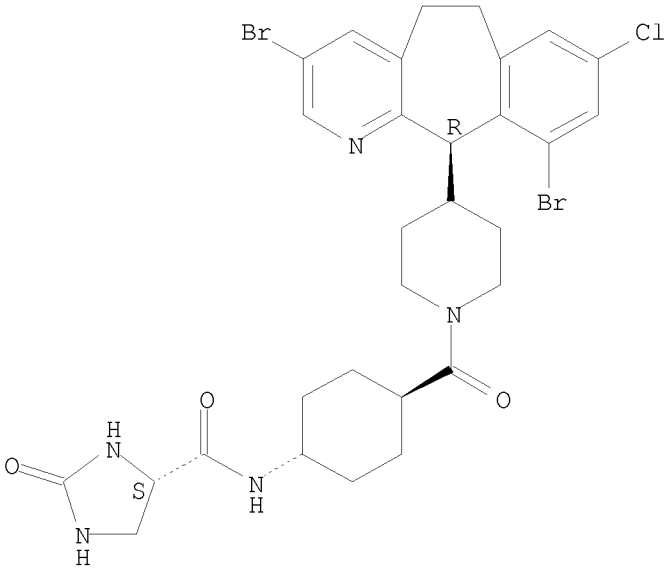
Absolute stereochemistry.



RN 218772-11-3 CAPLUS

CN 4-Imidazolidinecarboxamide, N-[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

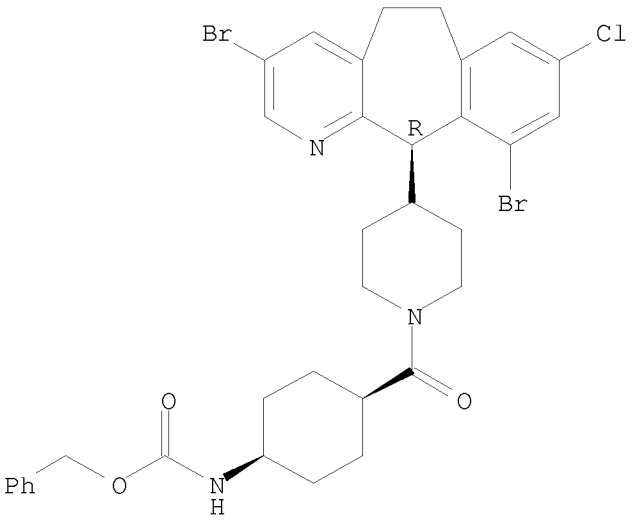
Absolute stereochemistry.



RN 218772-14-6 CAPLUS

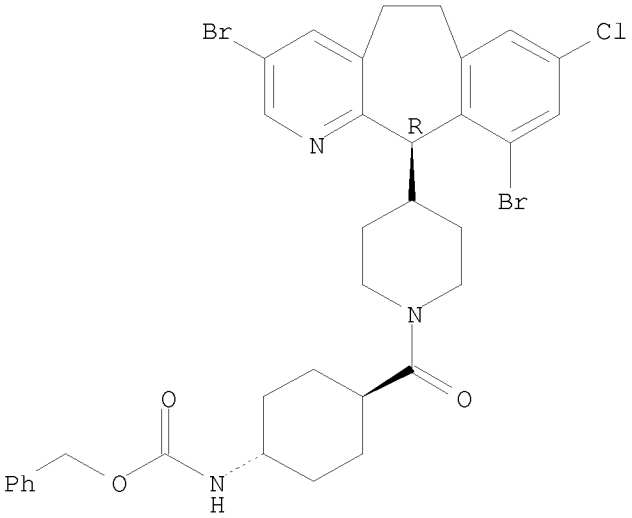
CN Carbamic acid, [cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



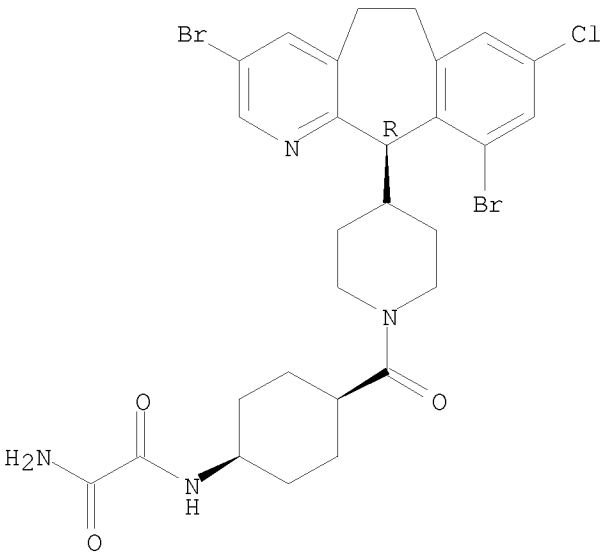
RN 218772-15-7 CAPLUS
CN Carbamic acid, [trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



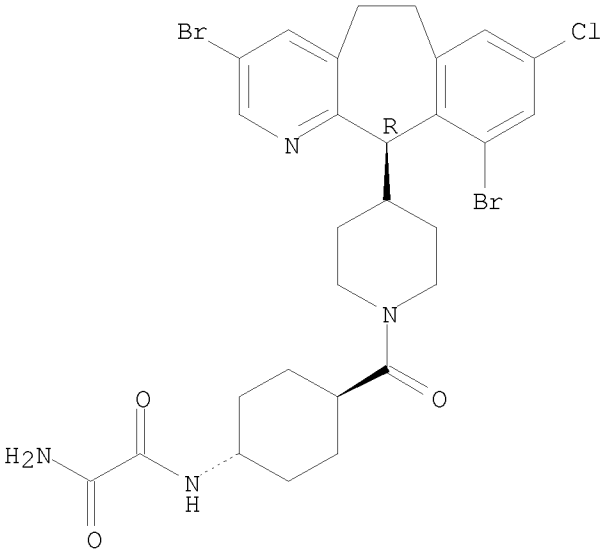
RN 218772-16-8 CAPLUS
CN Ethanediamide, N1-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



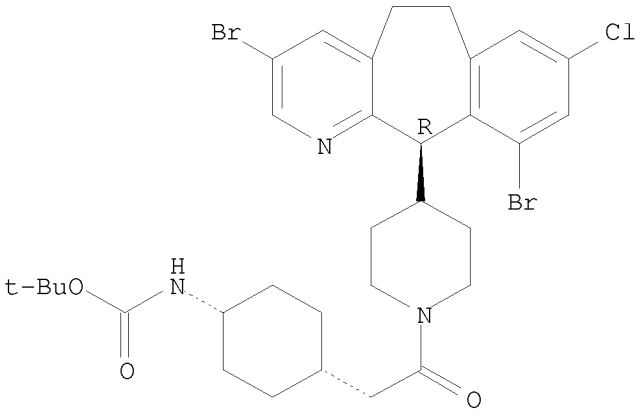
RN 218772-17-9 CAPLUS
CN Ethanediamide, N1-[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 218772-27-1 CAPLUS
CN Carbamic acid, [cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

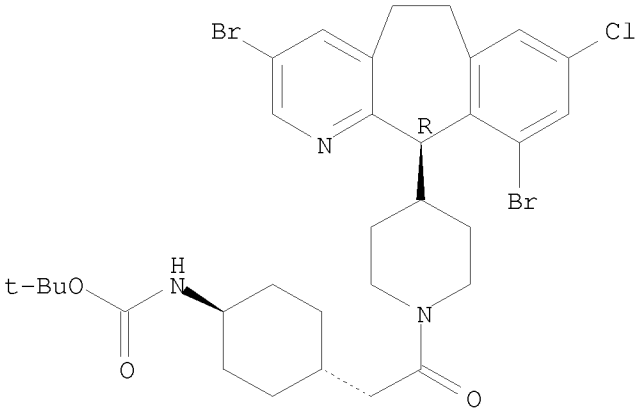
Absolute stereochemistry.



RN 218772-28-2 CAPLUS

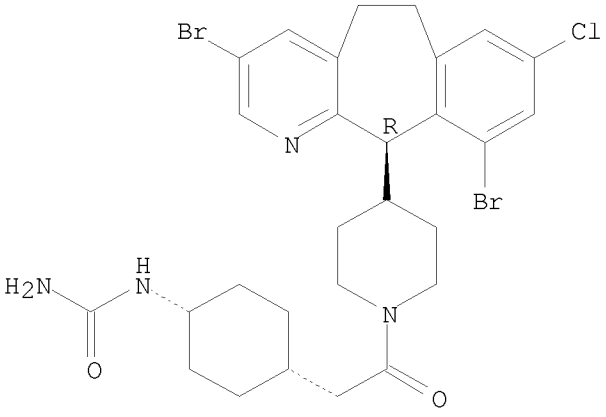
CN Carbamic acid, [trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



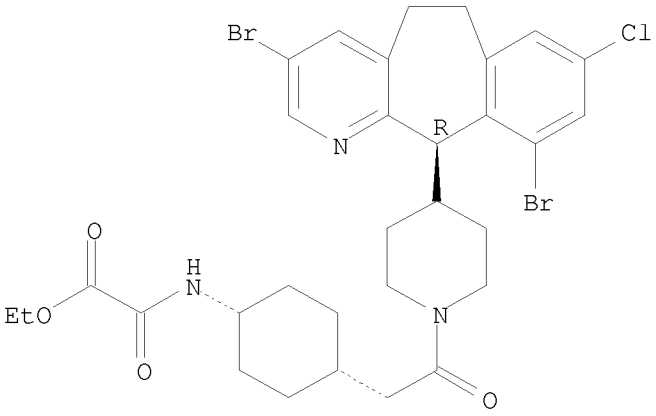
RN 218772-29-3 CAPLUS
CN Urea, N-[cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



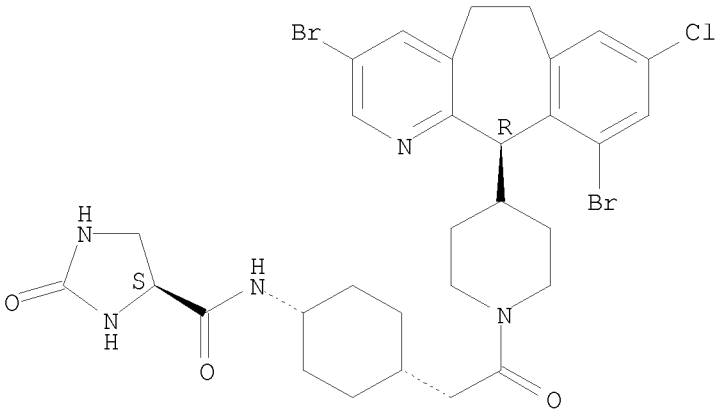
RN 218772-30-6 CAPLUS
CN Acetic acid, 2-[[cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



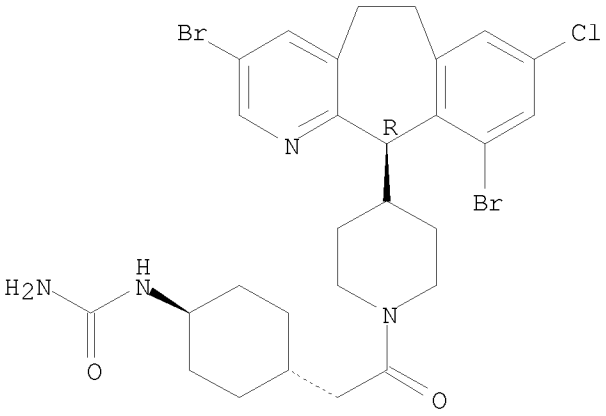
RN 218772-31-7 CAPLUS
CN 4-Imidazolidinecarboxamide, N-[cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



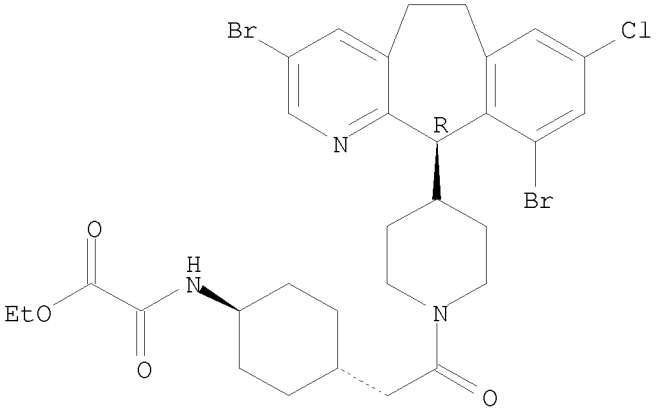
RN 218772-35-1 CAPLUS
CN Urea, N-[trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



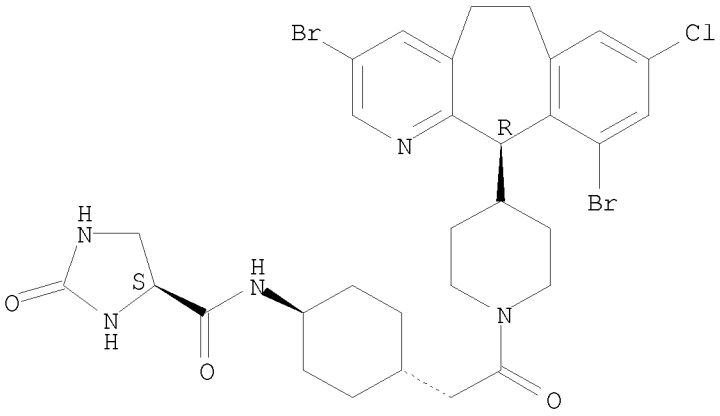
RN 218772-36-2 CAPLUS
CN Acetic acid, 2-[[trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



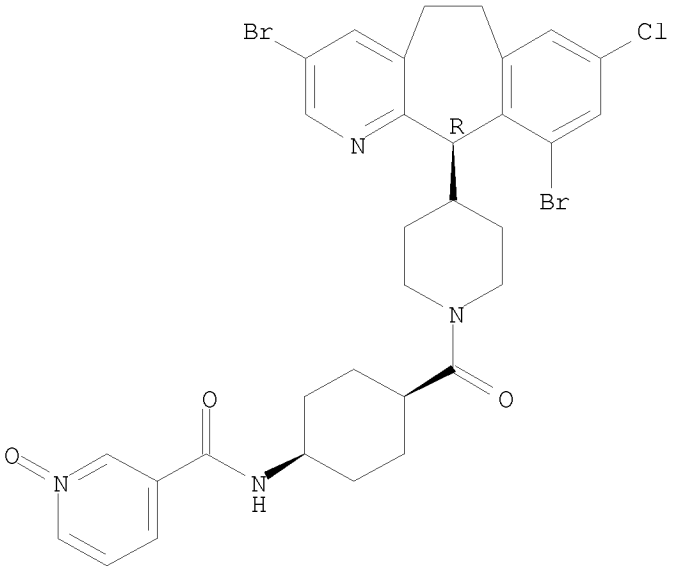
RN 218772-37-3 CAPLUS
CN 4-Imidazolidinecarboxamide, N-[trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



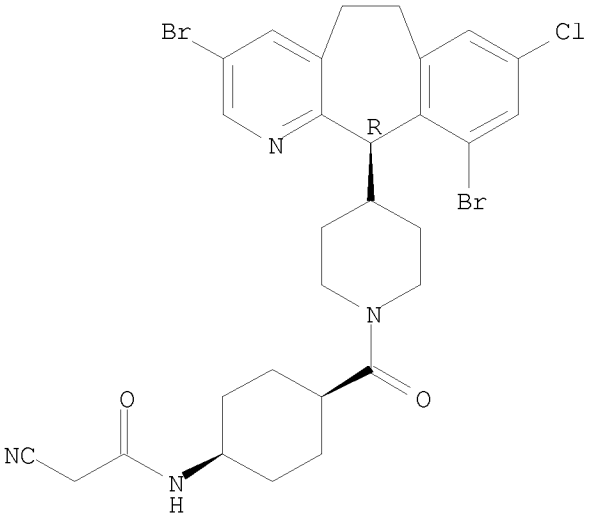
RN 218772-93-1 CAPLUS
CN 3-Pyridinecarboxamide, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1-oxide (CA INDEX NAME)

Absolute stereochemistry.



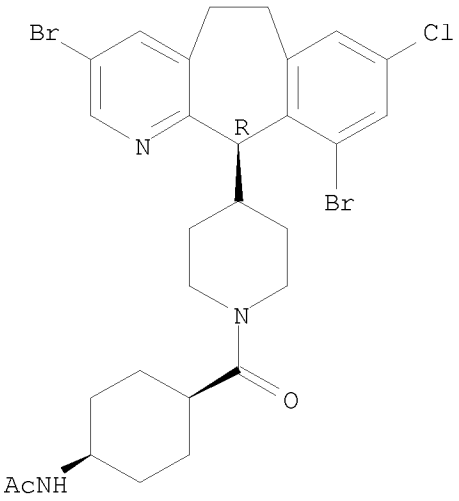
RN 218772-94-2 CAPLUS
CN Acetamide, 2-cyano-N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 218772-95-3 CAPLUS
CN Acetamide, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:614473 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 133:291015
TITLE: Acute and chronic administration of the selective D3 receptor antagonist SB-277011-A alters activity of

midbrain dopamine neurons in rats: an in vivo electrophysiological study

AUTHOR(S): Ashby, Charles R., Jr.; Minabe, Yoshio; Stemp, Geoff; Hagan, Jim J.; Middlemiss, Derek N.

CORPORATE SOURCE: Department of Pharmaceutical Health Sciences, College of Pharmacy and Allied Health Professions, St. John's University, Jamaica, NY, USA

SOURCE: Journal of Pharmacology and Experimental Therapeutics (2000), 294(3), 1166-1174
CODEN: JPETAB; ISSN: 0022-3565

PUBLISHER: American Society for Pharmacology and Experimental Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: English

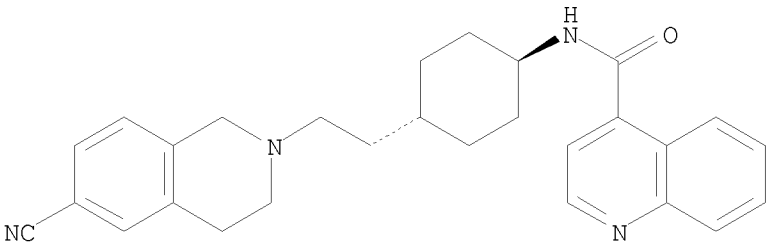
AB This study examined the effect of acute and repeated p.o. administration of the selective D3 receptor antagonist Smith-Kline Beecham (SB)-277011-A (1, 3, or 10 mg/kg) on the activity of spontaneously active midbrain dopamine (DA) neurons in anesthetized, male Sprague-Dawley rats. This was accomplished with the technique of in vivo extracellular single-unit recording. A single administration of either 3 or 10 mg/kg SB-277011-A produced a significant increase in the number of spontaneously active substantia nigra pars compacta (or A9) DA neurons compared with vehicle-treated (2% methylcellulose) animals. The 10-mg/kg dose of SB-277011-A produced a significant increase in the number of spontaneously active A10 DA neurons compared with vehicle-treated animals. The acute administration of SB-277011-A produced a significantly greater alteration in the firing pattern of spontaneously active A10 DA neurons, particularly at the 3- and 10-mg/kg doses, compared with vehicle-treated animals. The i.v. administration of SB-277011-A (0.01-1.28 mg/kg) did not significantly alter the firing rate or firing pattern of either A9 or A10 DA neurons. The repeated p.o. administration of 1, 3, or 10 mg/kg SB-277011-A once a day for 21 days produced a significant decrease in the number of spontaneously active A10 DA neurons. The repeated administration of SB-277011-A produced a greater effect on the firing pattern of spontaneously active A10 DA neurons, particularly at the 3-mg/kg dose, compared with A9 DA neurons. Overall, our results indicate that SB-277011-A alters the activity of midbrain DA neurons in rats.

IT 215803-78-4, SB-277011
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(acute and chronic administration of selective D3 receptor antagonist SB-277011-A alters activity of midbrain dopamine neurons in rats)

RN 215803-78-4 CAPLUS

CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

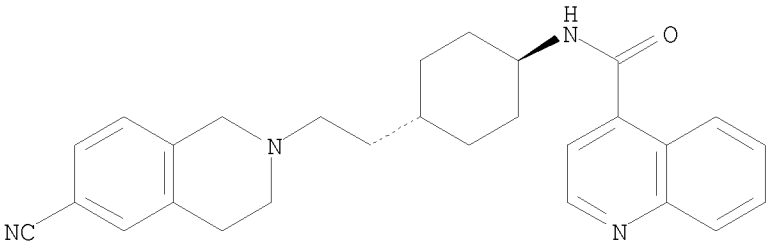
L18 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:614472 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 133:291014
TITLE: Pharmacological actions of a novel, high-affinity, and selective human dopamine D3 receptor antagonist, SB-277011-A
AUTHOR(S): Reavill, Charlie; Taylor, Stephen G.; Wood, Martyn D.; Ashmeade, Tracey; Austin, Nigel E.; Avenell, Kim Y.; Boyfield, Izzy; Branch, Clive L.; Cilia, Jackie; Coldwell, Martyn C.; Hadley, Michael S.; Hunter, A. Jackie; Jeffrey, Phil; Jewitt, Frances; Johnson, Christopher N.; Jones, Declan N. C.; Medhurst, Andrew D.; Middlemiss, Derek N.; Nash, David J.; Riley, Graham J.; Routledge, Carol; Stemp, Geoff; Thewlis, Kevin M.; Trail, Brenda; Vong, Antonio K. K.; Hagan, Jim J.
CORPORATE SOURCE: Department of Neuroscience Research, New Frontiers Science Park, SmithKline Beecham Pharmaceuticals, Harlow, UK
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2000), 294(3), 1154-1165
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB SB-277011-A {trans-N-[4-[2-(6-cyano-1,2,3,4-tetrahydroisoquinolin-2-yl)ethyl]cyclohexyl]-4-quinolininecarboxamide}, is a brain-penetrant, high-affinity, and selective dopamine D3 receptor antagonist. Radioligand-binding expts. in Chinese hamster ovary (CHO) cells transfected with human dopamine D3 or D2 long (hD3, hD2) receptors showed SB-277011-A to have high affinity for the hD3 receptor (pKi = 7.95) with 100-fold selectivity over the hD2 receptor and over 66 other receptors, enzymes, and ion channels. Similar radioligand-binding data for SB-277011-A were obtained from CHO cells transfected with rat dopamine D3 or D2. In the microphysiometer functional assay, SB-277011-A antagonized quinpirole-induced increases in acidification in CHO cells overexpressing the hD3 receptor (pKb = 8.3) and was 80-fold selective over hD2 receptors. Central nervous system penetration studies showed that SB-277011-A readily entered the brain. In in vivo microdialysis studies, SB-277011-A (2.8 mg/kg p.o.) reversed the quinelorane-induced reduction of dopamine efflux in

the nucleus accumbens but not striatum, a regional selectivity consistent with the distribution of the dopamine D3 receptor in rat brain. SB-277011-A (2-42.3 mg/kg p.o.) did not affect spontaneous locomotion, or stimulant-induced hyperlocomotion. SB-277011-A (4.1-42.2 mg/kg p.o.) did not reverse prepulse inhibition deficits in apomorphine- or quinpirole-treated rats, but did significantly reverse the prepulse inhibition deficit in isolation-reared rats at a dose of 3 mg/kg p.o. SB-277011-A (2.5-78.8 mg/kg p.o.) was noncataleptogenic and did not raise plasma prolactin levels. Thus, dopamine D3 receptor blockade produces few of the behavioral effects characteristic of nonselective dopamine receptor antagonists. The effect of SB-277011-A on isolation-induced prepulse inhibition deficit suggests that blockade of dopamine D3 receptors may benefit the treatment of schizophrenia.

IT 215803-78-4, SB 277011A
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(pharmacol. actions of a novel and high-affinity and selective human dopamine D3 receptor antagonist SB-277011-A in relation to central nervous system penetration and schizophrenia treatment)

RN 215803-78-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 23 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:291002 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 132:293678
TITLE: Preparation of tetrahydroisoquinolines as dopamine D3 modulators useful as antipsychotics.
INVENTOR(S): Johnson, Christopher Norbert; Stemp, Geoffrey
PATENT ASSIGNEE(S): Smithkline Beecham P.L.C., UK
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2000024717	A2	20000504	WO 1999-EP7761	19991006 <--
WO 2000024717	A3	20000914		
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1137638	A2	20011004	EP 1999-950729	19991006 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002528437	T	20020903	JP 2000-578287	19991006 <--
US 6358974	B1	20020319	US 2001-806875	20010703 <--
PRIORITY APPLN. INFO.:			GB 1998-21977 A	19981008 <--
			WO 1999-EP7761 W	19991006 <--

OTHER SOURCE(S): MARPAT 132:293678

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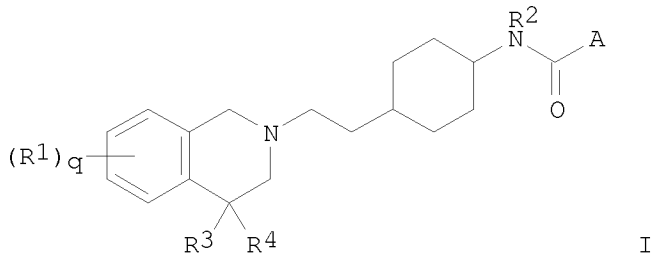


I

AB Title compds. [I; R1 = H, halo, OH, cyano, NO2, CF3, OCF3, SO2OCF3, C2F5, alkyl, alkoxy, aralkoxy, alkylthio, alkoxyalkyl, cycloalkylalkoxy, alkanoyl, alkoxycarbonyl, alkylsulfonyl, alkylsulfonyloxy, alkylsulfonylalkyl, arylsulfonyl, arylsulfonyloxy, arylsulfonylalkyl, alkylsulfonamido, alkylamido, alkylsulfonamidoalkyl, aroyl, aroylalkyl, aralkanoyl, etc.; R2 = H, alkyl; R3, R4 = alkyl; q = 1, 2; A = Ar, ArCH:CH, etc.; Ar = (substituted) Ph, 5-6 membered heteroaryl, bicyclic ring system], were prepared as antipsychotics (no data). Thus, I (R1, R2 = H; R3, R4 = Me; A = trans-4-FC6H4CH:CH) was prepared via coupling of trans-4-FC6H4CH:CHCO2H with the corresponding amine using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and cat. hydroxybenzotriazole in CH2Cl2.

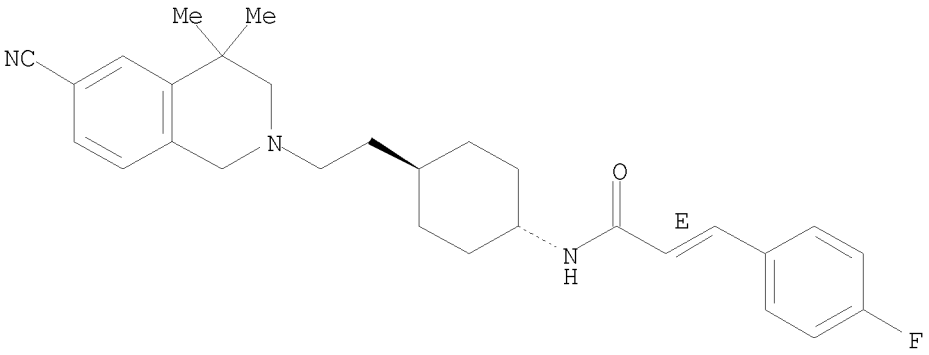
IT 264602-46-2P 264602-47-3P 264602-49-5P
264602-51-9P 264602-54-2P 264602-57-5P
264602-59-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tetrahydroisoquinolines as dopamine D3 modulators useful as antipsychotics)

RN 264602-46-2 CAPLUS

CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-fluorophenyl)-, (2E)- (CA INDEX NAME)

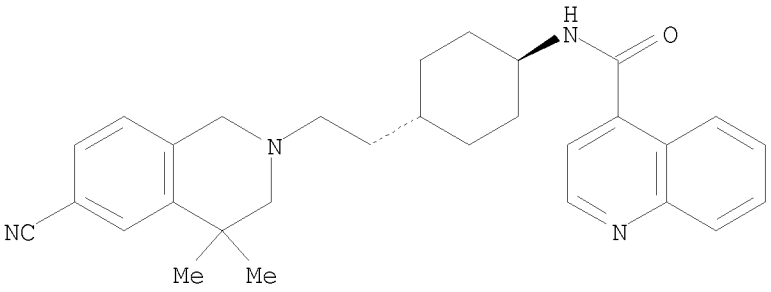
Relative stereochemistry.

Double bond geometry as shown.



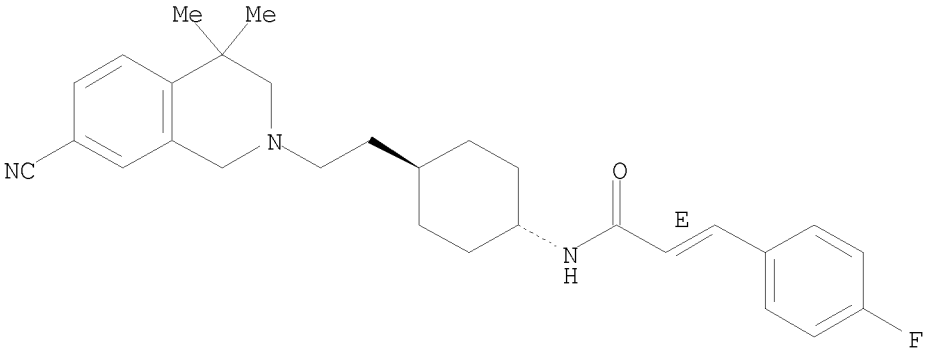
RN 264602-47-3 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



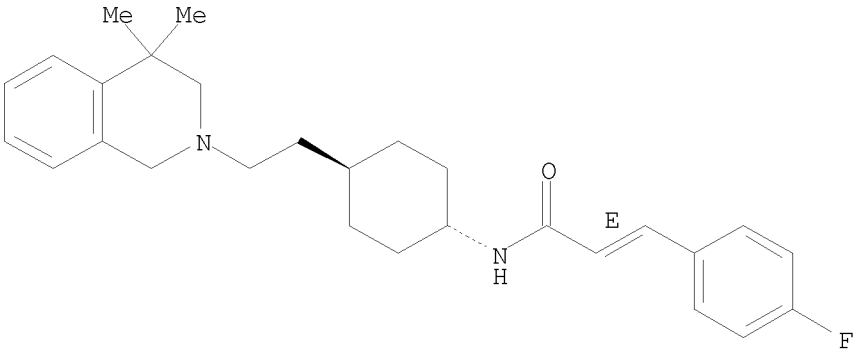
RN 264602-49-5 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-fluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



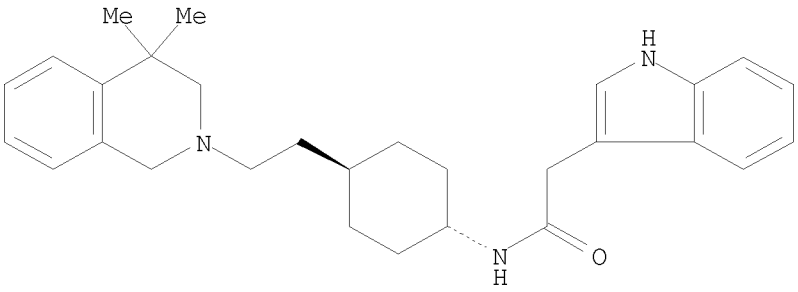
RN 264602-51-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-fluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



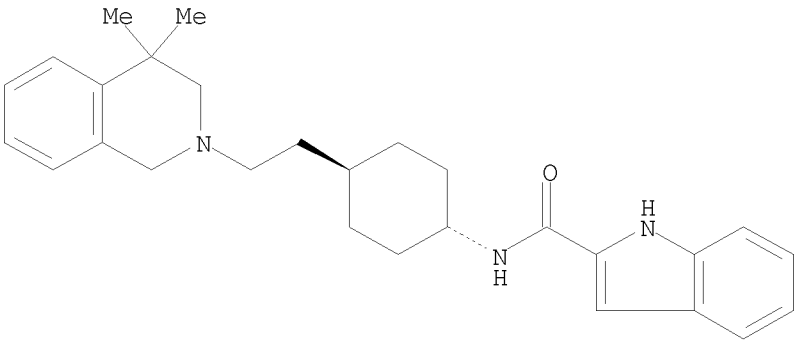
RN 264602-54-2 CAPLUS
CN 1H-Indole-3-acetamide, N-[trans-4-[2-(3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



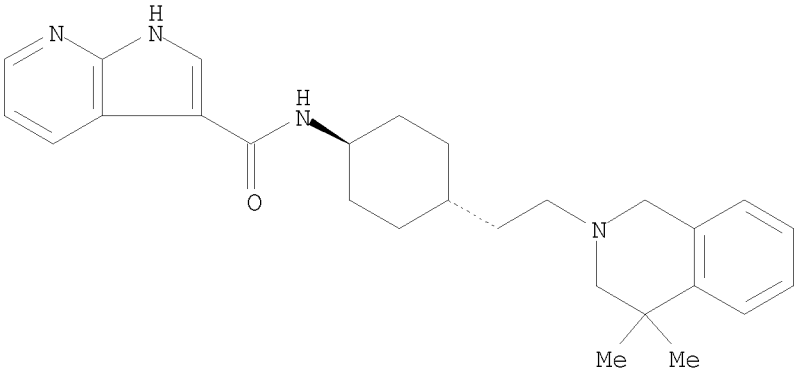
RN 264602-57-5 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



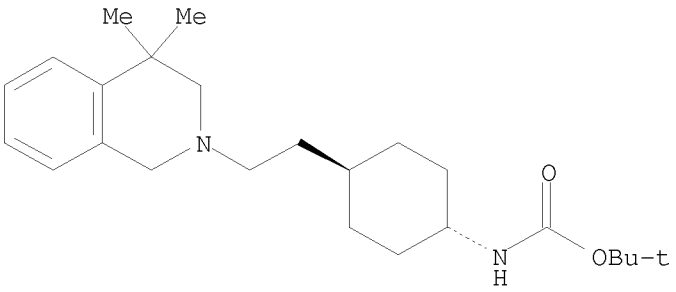
RN 264602-59-7 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine-3-carboxamide, N-[trans-4-[2-(3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



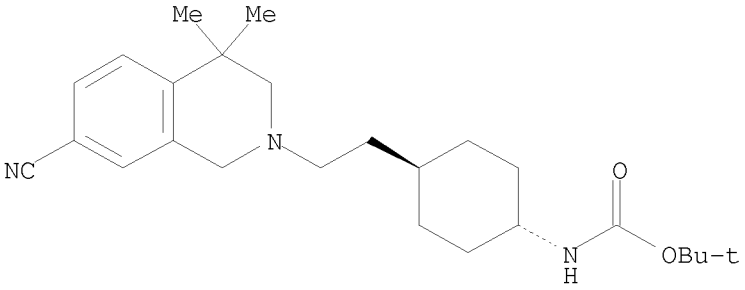
IT 264602-66-6P 264602-80-4P 264602-90-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrahydroisoquinolines as dopamine D3 modulators useful as antipsychotics)
RN 264602-66-6 CAPLUS
CN Carbamic acid, [trans-4-[2-(3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



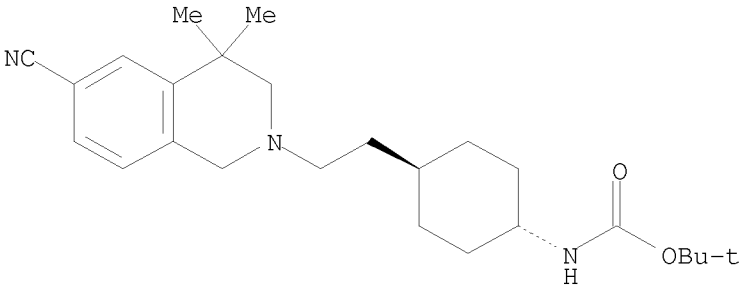
RN 264602-80-4 CAPLUS
CN Carbamic acid, [trans-4-[2-(7-cyano-3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 264602-90-6 CAPLUS
CN Carbamic acid, [trans-4-[2-(6-cyano-3,4-dihydro-4,4-dimethyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

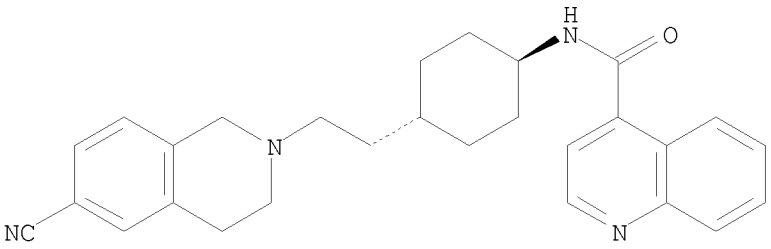
Relative stereochemistry.



L18 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:246722 CAPLUS <<LOGINID::20081022>>

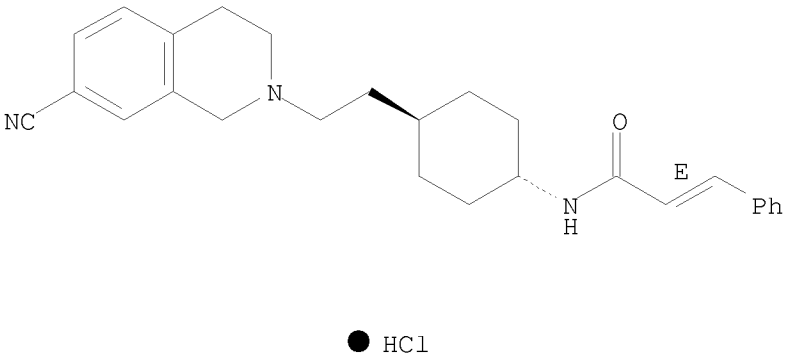
DOCUMENT NUMBER: 133:53147
TITLE: Design and Synthesis of trans-N-[4-[2-(6-Cyano-1,2,3,4-tetrahydroisoquinolin-2-yl)ethyl]cyclohexyl]-4-quinolinecarboxamide (SB-277011): A Potent and Selective Dopamine D3 Receptor Antagonist with High Oral Bioavailability and CNS Penetration in the Rat
AUTHOR(S): Stemp, Geoffrey; Ashmeade, Tracey; Branch, Clive L.; Hadley, Michael S.; Hunter, A. Jacqueline; Johnson, Christopher N.; Nash, David J.; Thewlis, Kevin M.; Vong, Antonio K. K.; Austin, Nigel E.; Jeffrey, Phillip; Avenell, Kim Y.; Boyfield, Izzy; Hagan, Jim J.; Middlemiss, Derek N.; Reavill, Charlie; Riley, Graham J.; Routledge, Carole; Wood, Martyn
CORPORATE SOURCE: Departments of Discovery Chemistry Neuroscience Research and Drug Metabolism and Pharmacokinetics, SmithKline Beecham Pharmaceuticals, Harlow, CM19 5AW, UK
SOURCE: Journal of Medicinal Chemistry (2000), 43(9), 1878-1885
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A selective dopamine D3 receptor antagonist offers the potential for an effective antipsychotic therapy, free of the serious side effects of currently available drugs. Using clearance and brain penetration studies as a screen, a series of 1,2,3,4-tetrahydroisoquinolines, exemplified by (I), was identified with high D3 affinity and selectivity against the D2 receptor. Following examination of mol. models, the flexible Bu linker present in I was replaced by a more conformationally constrained cyclohexylethyl linker, leading to compds. with improved oral bioavailability and selectivity over other receptors. Subsequent optimization of this new series to improve the cytochrome P 450 inhibitory profile and CNS penetration gave trans-N-[4-[2-(6-cyano-1,2,3,4-tetrahydroisoquinolin-2-yl)ethyl]cyclohexyl]-4-quinolinecarboxamide (SB-277011). This compound is a potent and selective dopamine D3 receptor antagonist with high oral bioavailability and brain penetration in the rat and represents an excellent new chemical tool for the investigation of the role of the dopamine D3 receptor in the CNS.
IT 215803-78-4P, SB 277011 276689-95-3P 276689-96-4P 276689-97-5P 276689-98-6P 276689-99-7P 276690-00-7P 276690-01-8P 276690-02-9P 276690-03-0P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation and structure activity relations of quinolinecarboxamides as dopamine D3 antagonists as oral bioavailability and transport to brain)
RN 215803-78-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 276689-95-3 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

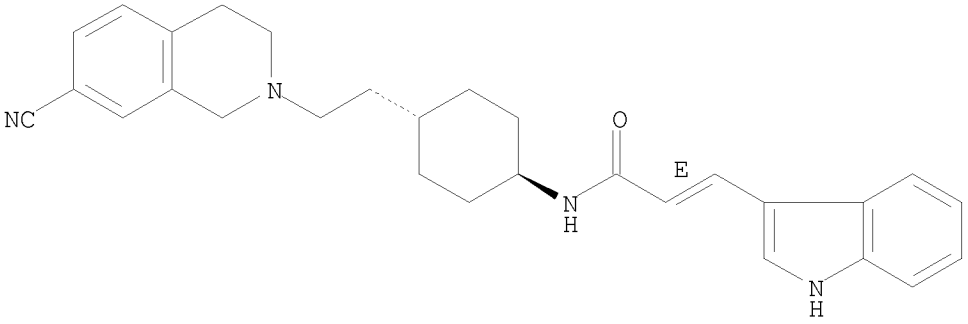
Relative stereochemistry.
Double bond geometry as shown.



● HCl

RN 276689-96-4 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(1H-indol-3-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

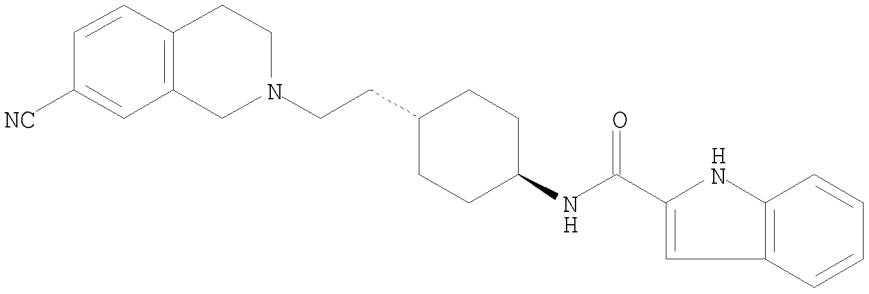
Relative stereochemistry.
Double bond geometry as shown.



● HCl

RN 276689-97-5 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

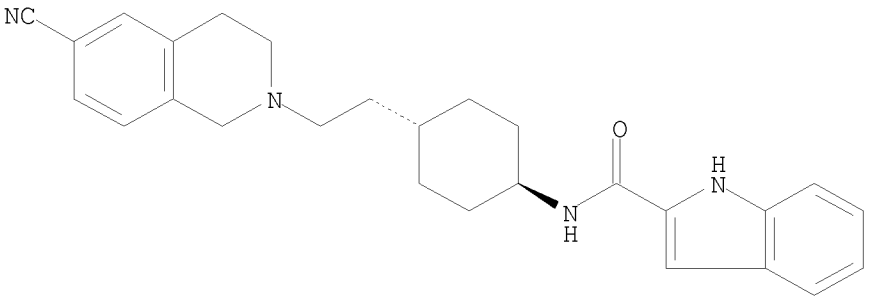
Relative stereochemistry.



● HCl

RN 276689-98-6 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

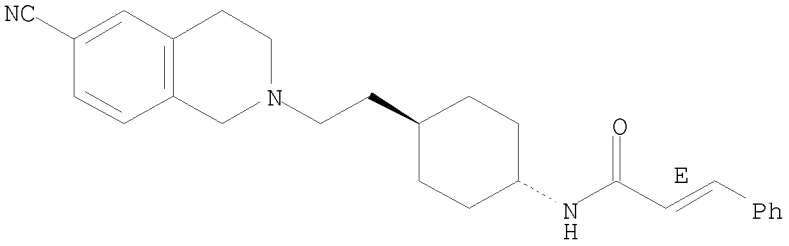
Relative stereochemistry.



● HCl

RN 276689-99-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

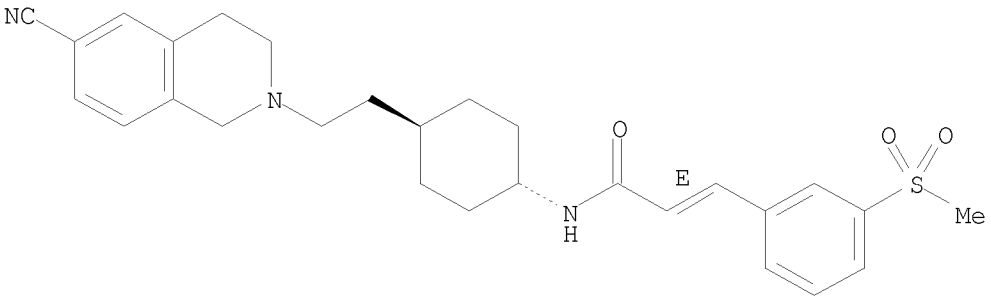
Relative stereochemistry.
Double bond geometry as shown.



● HCl

RN 276690-00-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[3-(methylsulfonyl)phenyl]-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

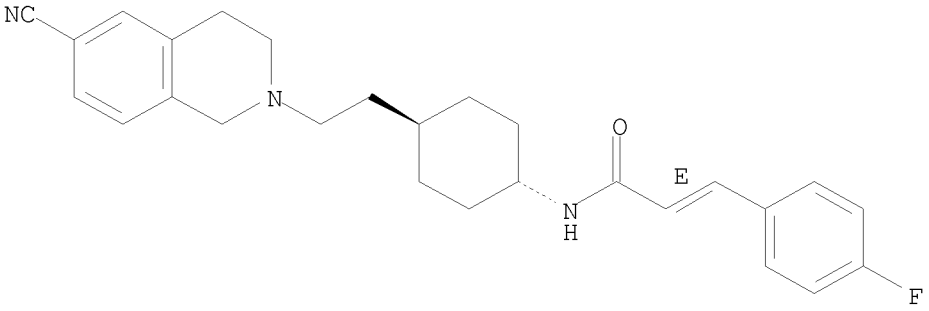
Relative stereochemistry.
Double bond geometry as shown.



● HCl

RN 276690-01-8 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-fluorophenyl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

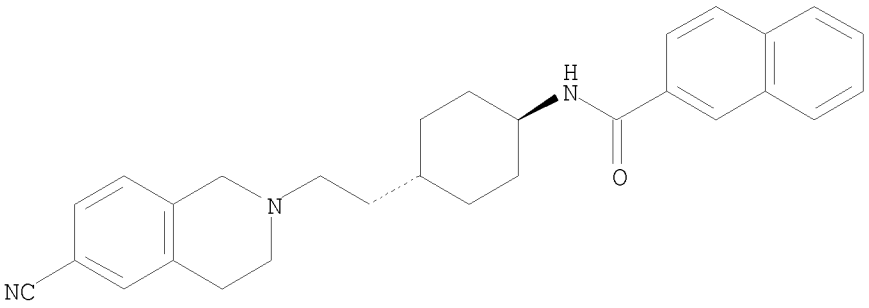
Relative stereochemistry.
Double bond geometry as shown.



● HCl

RN 276690-02-9 CAPLUS
CN 2-Naphthalenecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

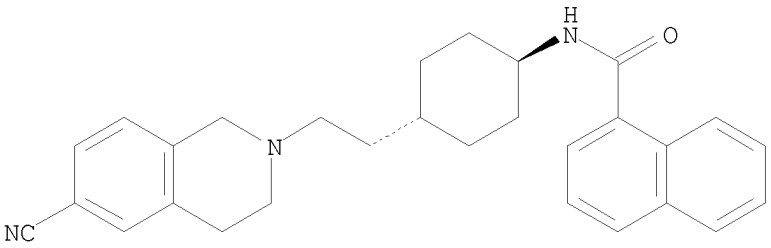
Relative stereochemistry.



● HCl

RN 276690-03-0 CAPLUS
CN 1-Naphthalenecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

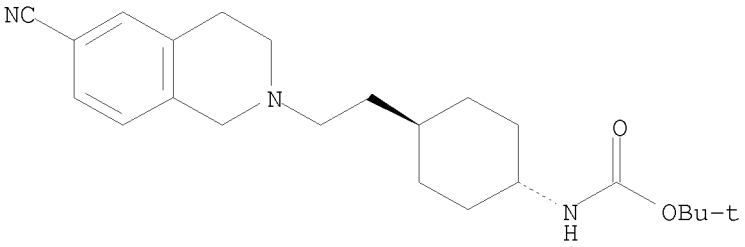
Relative stereochemistry.



● HCl

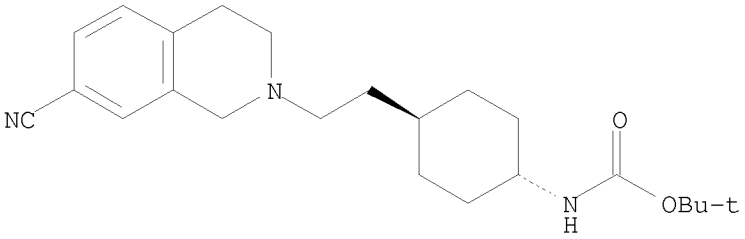
IT 215790-38-8P 215790-43-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure activity relations of quinolinecarboxamides as dopamine D3 antagonists as oral bioavailability and transport to brain)
RN 215790-38-8 CAPLUS
CN Carbamic acid, [trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



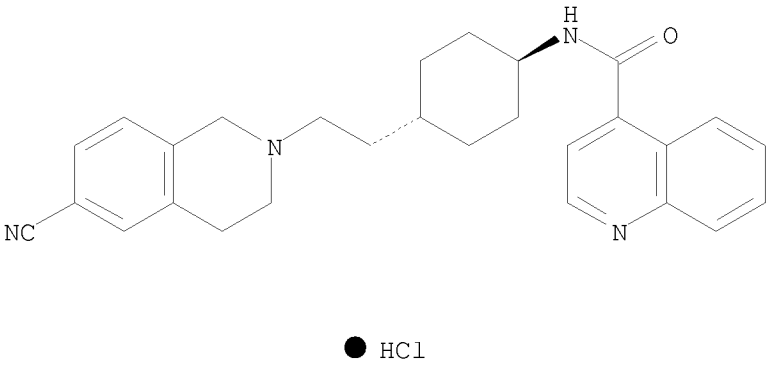
RN 215790-43-5 CAPLUS
CN Carbamic acid, [trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 215804-67-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and structure activity relations of quinolinecarboxamides as dopamine D3 antagonists as oral bioavailability and transport to brain)
RN 215804-67-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.



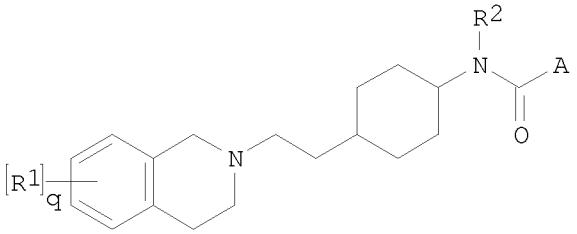
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:795805 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 132:35623
TITLE: Preparation of tetrahydroisoquinolines as modulators of dopamine D3 receptors
INVENTOR(S): Branch, Clive Leslie; Johnson, Christopher Norbert; Stemp, Geoffrey
PATENT ASSIGNEE(S): Smithkline Beecham P.L.C., UK
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964412	A1	19991216	WO 1999-EP3840	19990601 <--
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2334814	A1	19991216	CA 1999-2334814	19990601 <--
EP 1086095	A1	20010328	EP 1999-926510	19990601 <--
EP 1086095	B1	20021023		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2002517493	T	20020618	JP 2000-553421	19990601 <--
ES 2186365	T3	20030501	ES 1999-926510	19990601 <--
US 20030191314	A1	20031009	US 2003-367306	20030214 <--
US 6855717	B2	20050215		

PRIORITY APPLN. INFO.:	GB 1998-12522	A	19980610 <--
	WO 1999-EP3840	W	19990601 <--
	US 2000-719146	B1	20001207 <--

OTHER SOURCE(S): MARPAT 132:35623
GI



I

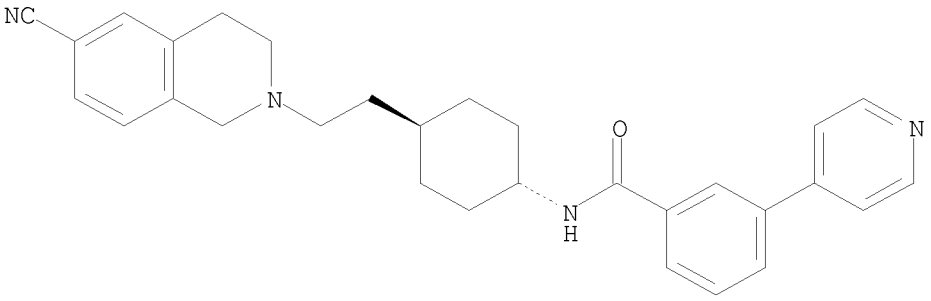
AB The title compds. [I; R1 = H, halo, OH, etc.; R2 = H, alkyl; q = 1-2; A = II, III (wherein T, U, V, Y = CH, N; R5 = H, halo, CN, etc.; s = 1-2; Ar2 = (un)substituted Ph, 5-6 membered heteroaryl)], useful for the treatment

of conditions which require modulation of a dopamine receptor such as schizophrenia, were prepared and formulated. Thus, reacting trans-2-{2-[1-(4-amino)cyclohexyl]ethyl}-6-cyano-1,2,3,4-tetrahydroisoquinoline (preparation given) with 3-(4-pyridyl)benzoic acid in the presence of 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide.HCl and 1-hydroxybenzotriazole in CH2Cl2 afforded 46% I trans-[R1 = 6-CN; R2 = H; A = 3-(4-pyridyl)phenyl]. Compds. I are effective at 0.1-50 mg/day for an adult patient.

IT 252331-56-9P 252331-57-0P 252331-58-1P
252331-59-2P 252331-60-5P 252331-61-6P
252331-62-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tetrahydroisoquinolines as modulators of dopamine D3 receptors)

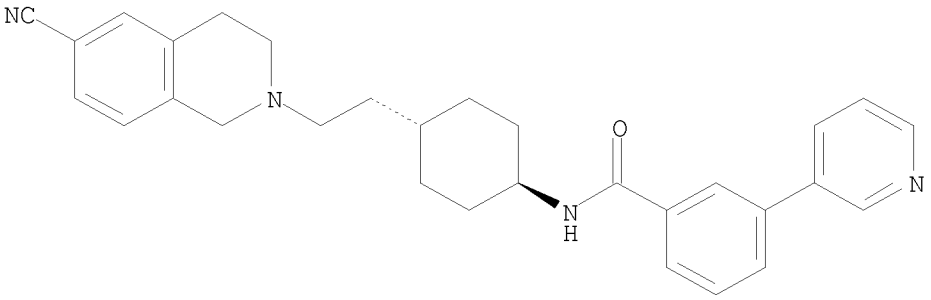
RN 252331-56-9 CAPLUS
CN Benzamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-pyridinyl)- (CA INDEX NAME)

Relative stereochemistry.



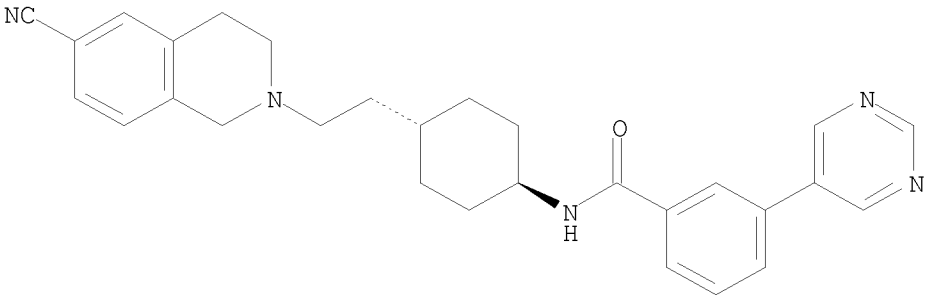
RN 252331-57-0 CAPLUS
CN Benzamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3-pyridinyl)- (CA INDEX NAME)

Relative stereochemistry.



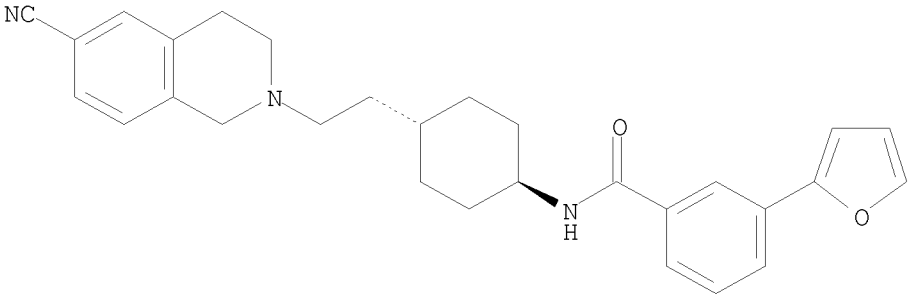
RN 252331-58-1 CAPLUS
CN Benzamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(5-pyrimidinyl)- (CA INDEX NAME)

Relative stereochemistry.



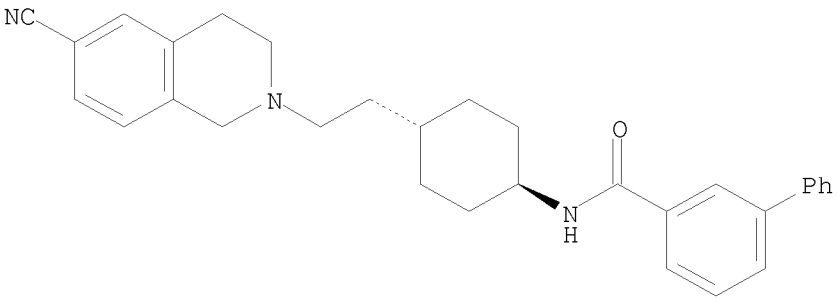
RN 252331-59-2 CAPLUS
CN Benzamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-furanyl)- (CA INDEX NAME)

Relative stereochemistry.



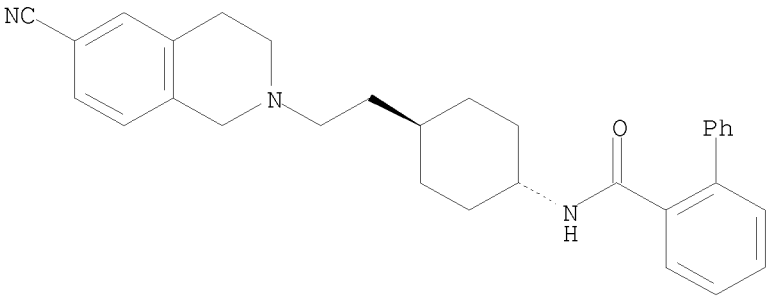
RN 252331-60-5 CAPLUS
CN [1,1'-Biphenyl]-3-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



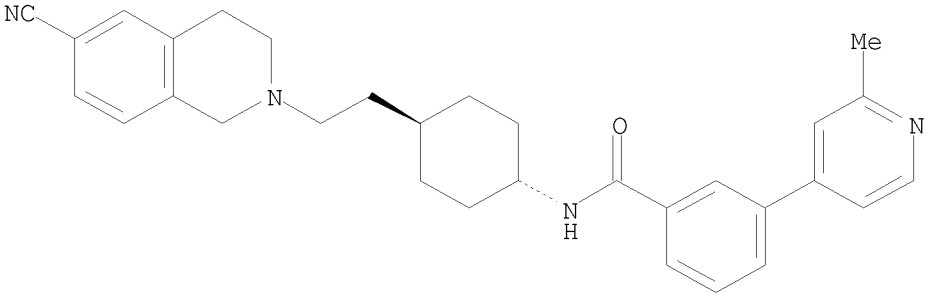
RN 252331-61-6 CAPLUS
CN [1,1'-Biphenyl]-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 252331-62-7 CAPLUS
CN Benzamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-methyl-4-pyridinyl)- (CA INDEX NAME)

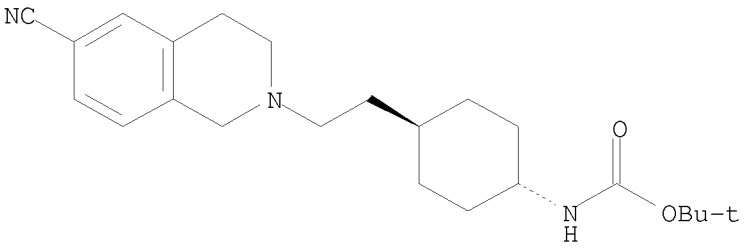
Relative stereochemistry.



IT 215790-38-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of tetrahydroisoquinolines as modulators of dopamine D3 receptors)
RN 215790-38-8 CAPLUS
CN Carbamic acid, [trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

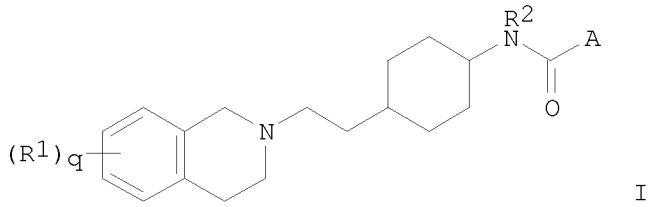


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:753214 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 132:3322
TITLE: Preparation of acylaminocyclohexylethyltetrahydroisoquinolines as modulators of dopamine D3 receptors
INVENTOR(S): Vong, Antonio Kuok Keong
PATENT ASSIGNEE(S): SmithKline Beecham PLC, UK
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9959974	A1	19991125	WO 1999-EP3371	19990514 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2332316	A1	19991125	CA 1999-2332316	19990514 <--
AU 9942627	A	19991206	AU 1999-42627	19990514 <--
EP 1086084	A1	20010328	EP 1999-952090	19990514 <--
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2002515489	T	20020528	JP 2000-549593	19990514 <--

US 6414154 B1 20020702 US 2001-700775 20010316 <--
PRIORITY APPLN. INFO.: GB 1998-10876 A 19980520 <--
WO 1999-EP3371 W 19990514 <--
OTHER SOURCE(S): MARPAT 132:3322
GI



I

AB Title compds. [I; R1 = H, halo, OH, cyano, NO2, CF3, OCF3, F3CSO2O, pentafluoroethyl, alkyl, alkoxy, aralkoxy, alkylthio, alkoxyalkyl, cycloalkylalkoxy, alkanoyl, alkoxycarbonyl, alkylsulfonyl, alkylsulfonyloxy, alkylsulfonylalkyl, arylsulfonyl, arylsulfonyloxy, etc.; R2 = H, alkyl; q = 1, 2; A = (CH2)rV(CH2)sAr; r, s = 0- 3; r+s = 1-4; V = bond, O, S; Ar = (substituted) Ph, 5-6 membered heteroaryl, bicyclyl], were prepared Thus, trans-2-[2-[1-(4-phenylacetamido)cyclohexyl]ethyl]-1,2,3,4-tetrahydroisoquinoline (preparation given), phenylacetic acid, 1-hydroxybenzotriazole, and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride were stirred 16 h in CH2Cl2 to give 64% trans-6-cyano-2-[2-[1-(4-phenylacetamido)cyclohexyl]ethyl]-1,2,3,4-tetrahydroisoquinoline. I bound to D3 receptors with pKi = 7.9-8.5.

IT 250777-93-6P 250777-94-7P 250777-95-8P
250777-96-9P 250777-97-0P 250777-98-1P
250777-99-2P 250778-00-8P 250778-01-9P
250778-02-0P 250778-03-1P 250778-04-2P
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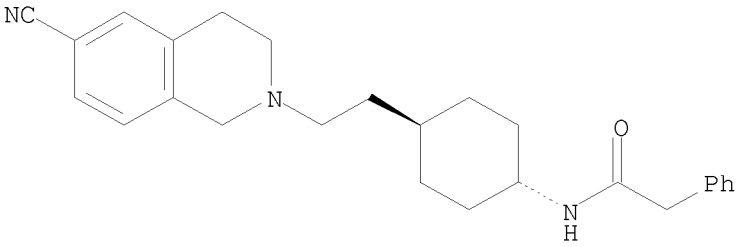
250778-17-7P 250778-18-8P 250778-19-9P
250778-20-2P 250778-21-3P 250778-22-4P
250778-23-5P 250778-24-6P 250778-25-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acylaminocyclohexylethyltetrahydroisoquinolines as modulators of dopamine D3 receptors)

RN 250777-93-6 CAPLUS

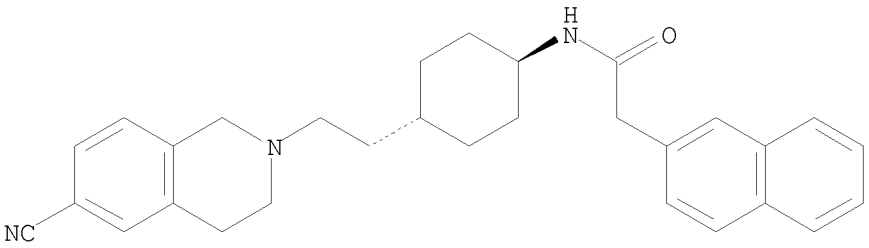
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



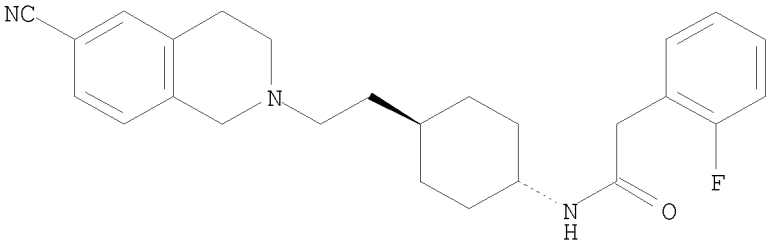
RN 250777-94-7 CAPLUS
CN 2-Naphthaleneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



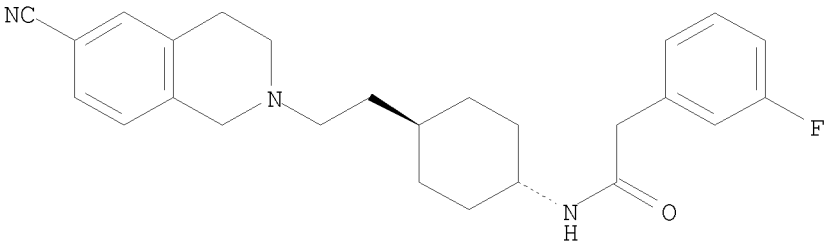
RN 250777-95-8 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2-fluoro- (CA INDEX NAME)

Relative stereochemistry.



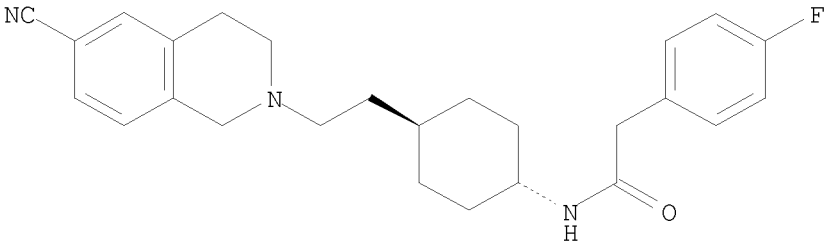
RN 250777-96-9 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-fluoro- (CA INDEX NAME)

Relative stereochemistry.



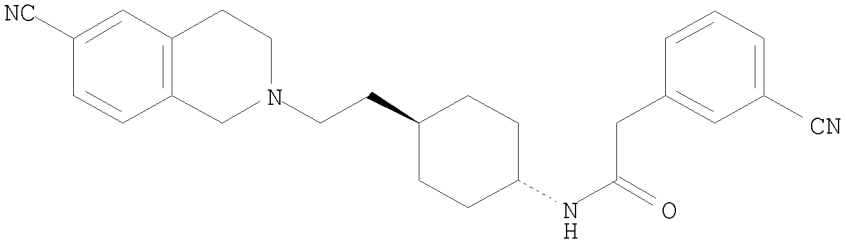
RN 250777-97-0 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-fluoro- (CA INDEX NAME)

Relative stereochemistry.



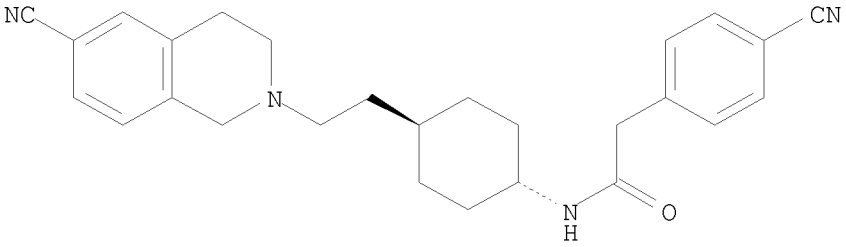
RN 250777-98-1 CAPLUS
CN Benzeneacetamide, 3-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



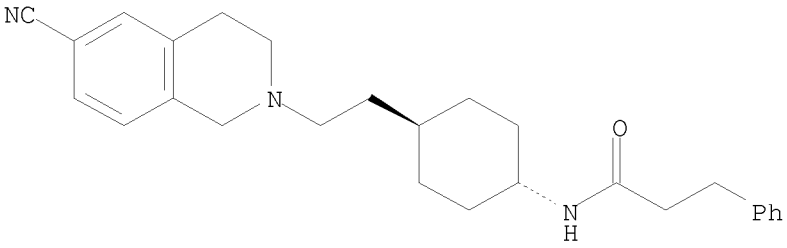
RN 250777-99-2 CAPLUS
CN Benzeneacetamide, 4-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



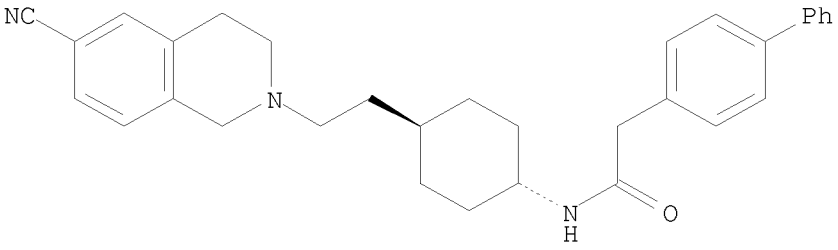
RN 250778-00-8 CAPLUS
CN Benzenepropanamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



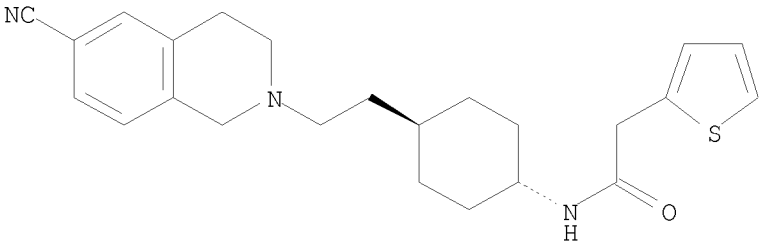
RN 250778-01-9 CAPLUS
CN [1,1'-Biphenyl]-4-acetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



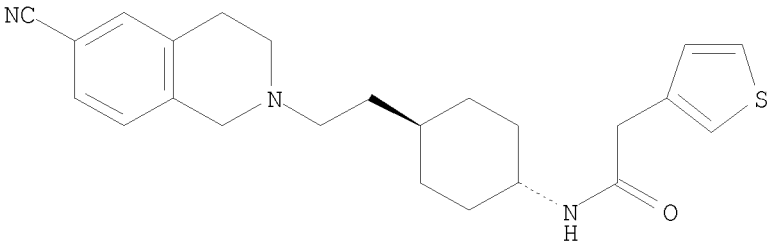
RN 250778-02-0 CAPLUS
CN 2-Thiopheneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



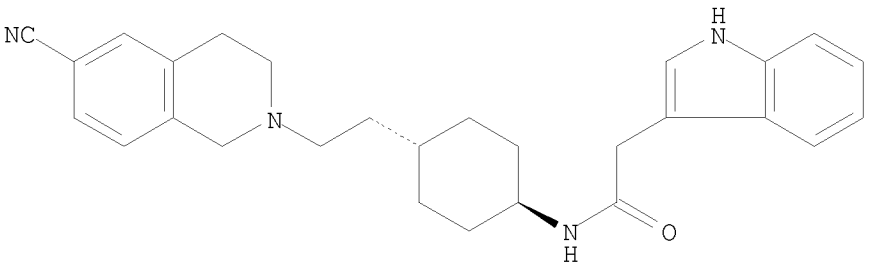
RN 250778-03-1 CAPLUS
CN 3-Thiopheneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



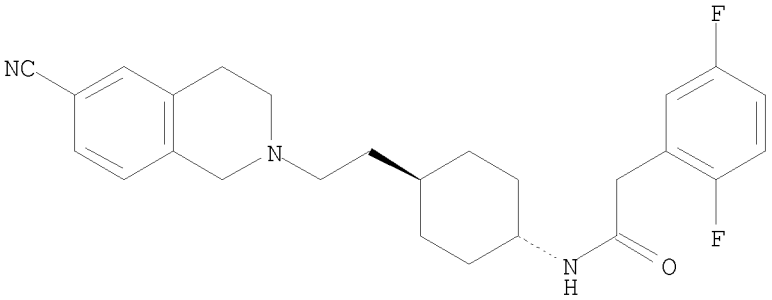
RN 250778-04-2 CAPLUS
CN 1H-Indole-3-acetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



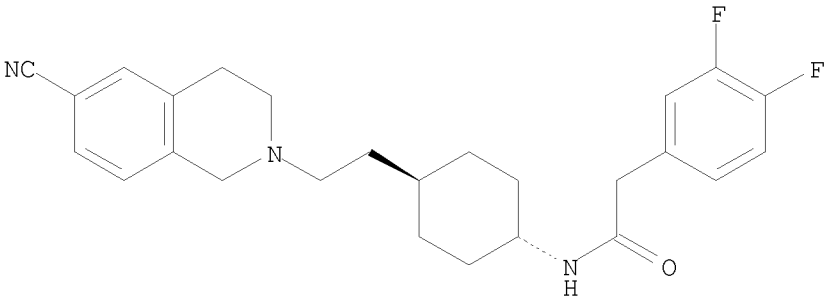
RN 250778-05-3 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2,5-difluoro- (CA INDEX NAME)

Relative stereochemistry.



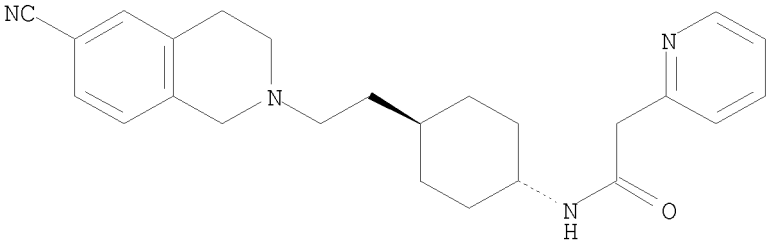
RN 250778-06-4 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3,4-difluoro- (CA INDEX NAME)

Relative stereochemistry.



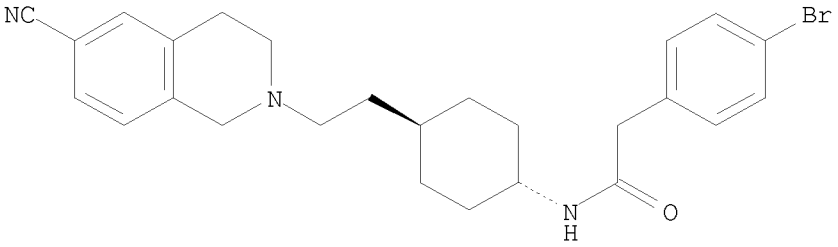
RN 250778-07-5 CAPLUS
CN 2-Pyridineacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



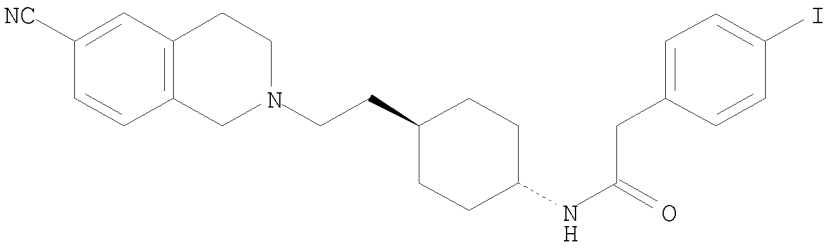
RN 250778-08-6 CAPLUS
CN Benzeneacetamide, 4-bromo-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



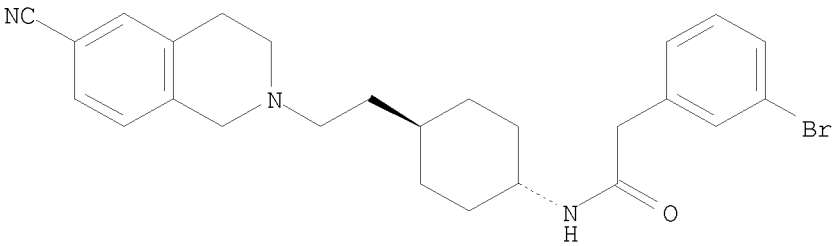
RN 250778-09-7 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-iodo- (CA INDEX NAME)

Relative stereochemistry.



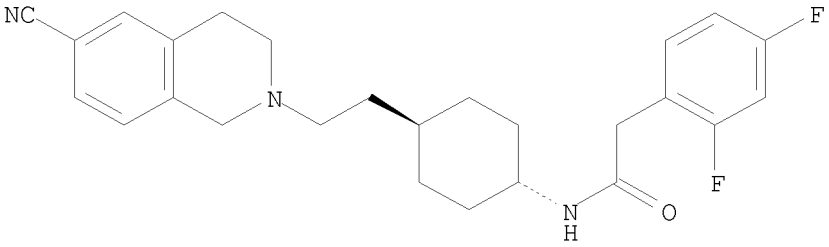
RN 250778-10-0 CAPLUS
CN Benzeneacetamide, 3-bromo-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



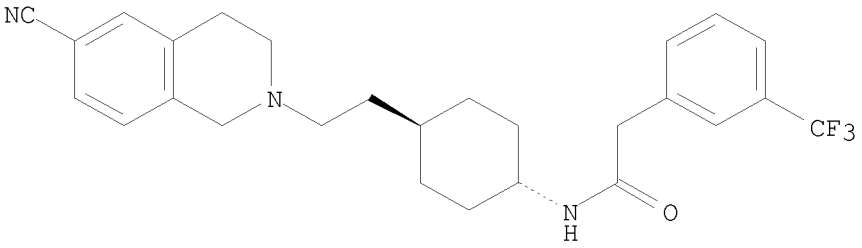
RN 250778-11-1 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2,4-difluoro- (CA INDEX NAME)

Relative stereochemistry.



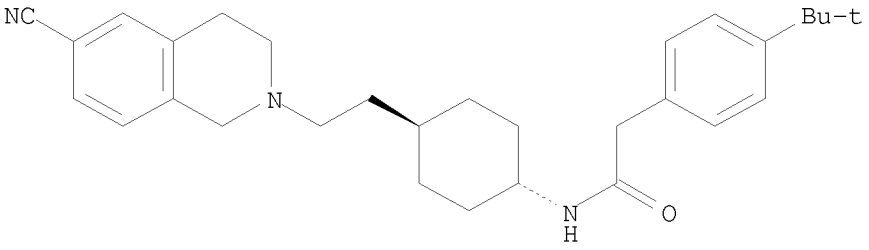
RN 250778-12-2 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(trifluoromethyl)- (CA INDEX NAME)

Relative stereochemistry.



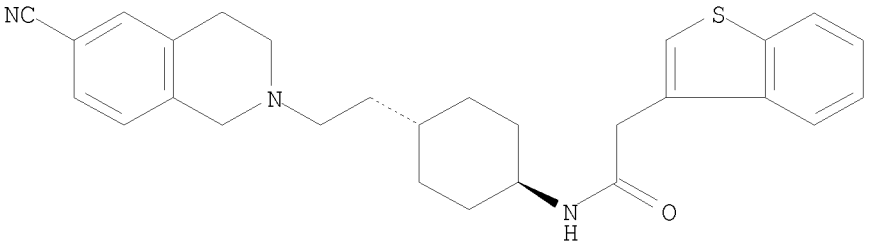
RN 250778-13-3 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-(1,1-dimethylethyl)- (CA INDEX NAME)

Relative stereochemistry.



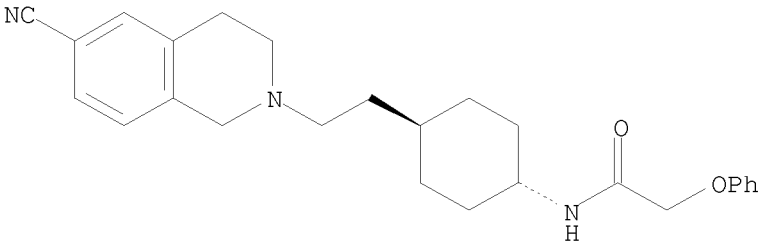
RN 250778-14-4 CAPLUS
CN Benzo[b]thiophene-3-acetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



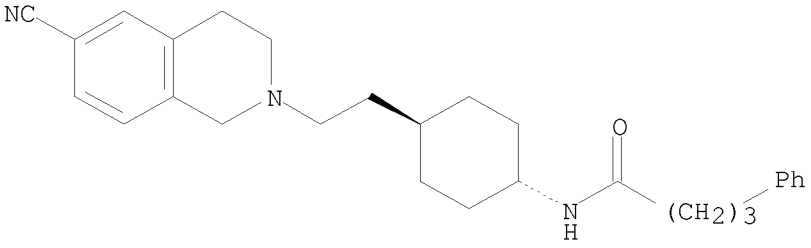
RN 250778-15-5 CAPLUS
CN Acetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2-phenoxy- (CA INDEX NAME)

Relative stereochemistry.



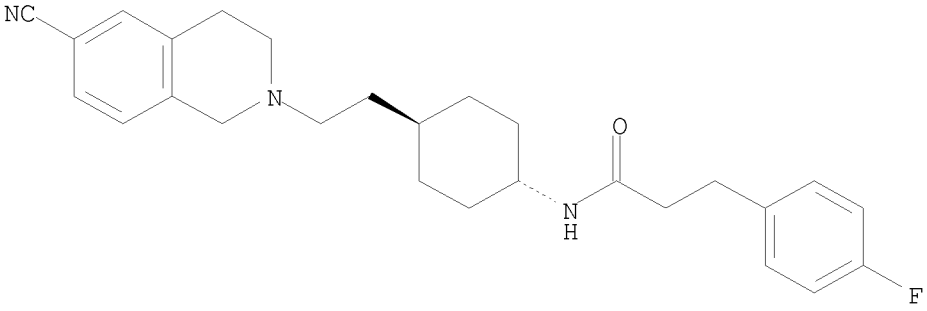
RN 250778-16-6 CAPLUS
CN Benzenebutanamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



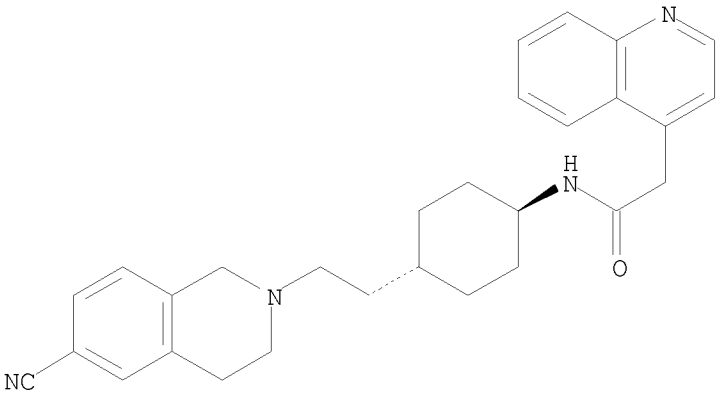
RN 250778-17-7 CAPLUS
CN Benzenepropanamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-fluoro- (CA INDEX NAME)

Relative stereochemistry.



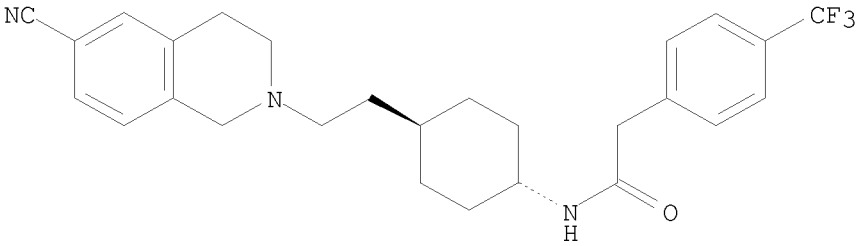
RN 250778-18-8 CAPLUS
CN 4-Quinolineacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 250778-19-9 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-(trifluoromethyl)- (CA INDEX NAME)

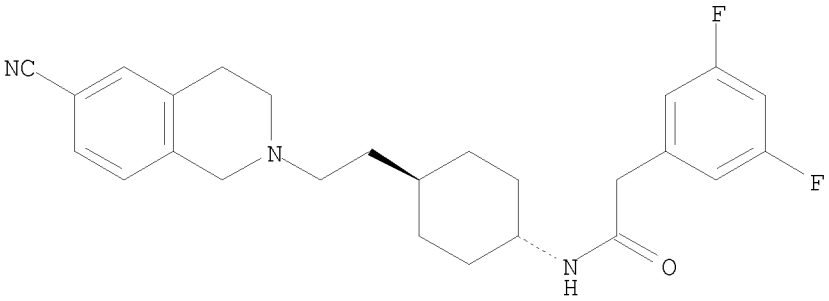
Relative stereochemistry.



RN 250778-20-2 CAPLUS

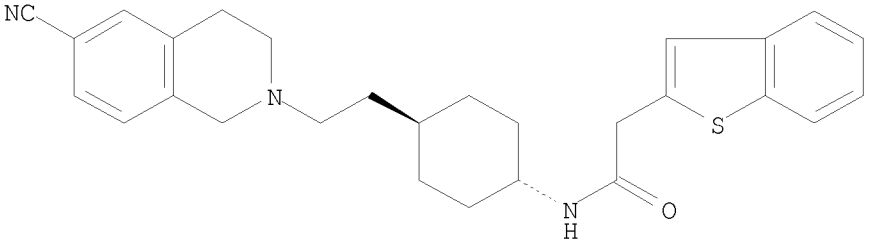
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3,5-difluoro- (CA INDEX NAME)

Relative stereochemistry.



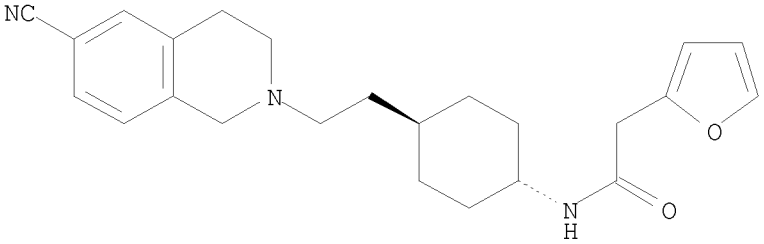
RN 250778-21-3 CAPLUS
CN Benzo[b]thiophene-2-acetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 250778-22-4 CAPLUS
CN 2-Furanacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

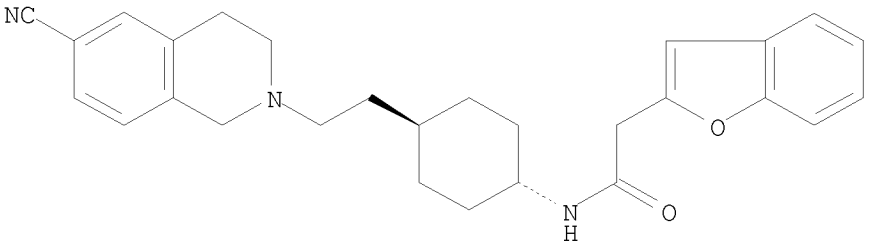
Relative stereochemistry.



RN 250778-23-5 CAPLUS

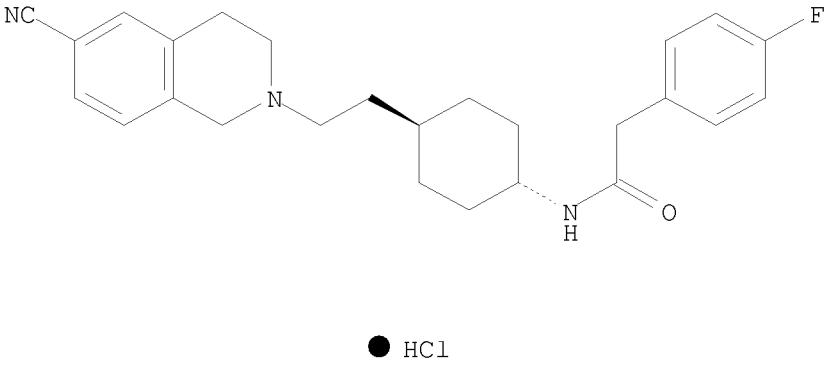
CN 2-Benzofuranacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



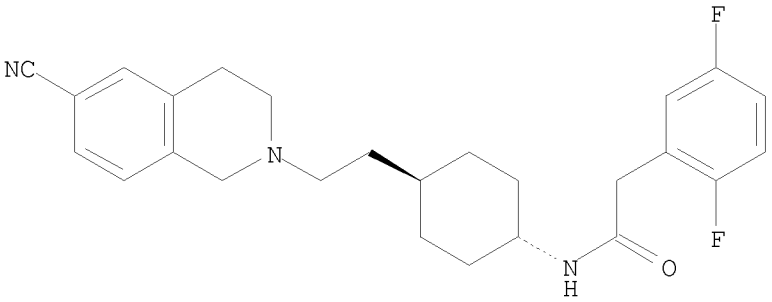
RN 250778-24-6 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-fluoro-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.



RN 250778-25-7 CAPLUS
CN Benzeneacetamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2,5-difluoro-, hydrochloride (1:1) (CA INDEX NAME)

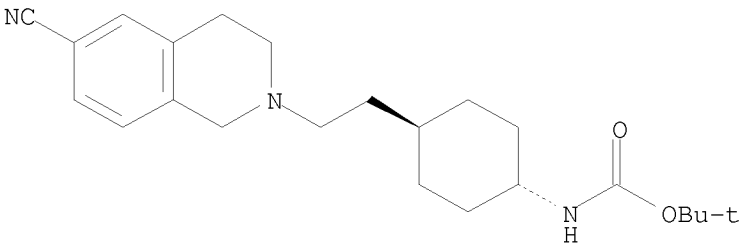
Relative stereochemistry.



● HCl

IT 215790-38-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acylaminocyclohexylethyltetrahydroisoquinolines as modulators of dopamine D3 receptors)
RN 215790-38-8 CAPLUS
CN Carbamic acid, [trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:9837 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 130:81410
TITLE: Preparation of 11-piperidinylbenzo[5,6]cyclohepta[1,2-b]pyridines and related compounds as inhibitors of farnesyl protein transferase.
INVENTOR(S): Remiszewski, Stacy W.; Doll, Ronald J.; Alvarez, Carmen
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 9857955	A1	19981223	WO 1998-US11494		19980615	<--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UZ, VN, YU						
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG						
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CA 2294351	C	20080902				
AU 9878151	A	19990104	AU 1998-78151		19980615	<--
EP 993459	A1	20000419	EP 1998-926276		19980615	<--
EP 993459	B1	20021106				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, LT, LV, FI, RO						
HU 2000002186	A2	20010428	HU 2000-2186		19980615	<--
HU 2000002186	A3	20020429				
JP 2002504143	T	20020205	JP 1999-504489		19980615	<--
AT 227281	T	20021115	AT 1998-926276		19980615	<--
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MX 9912090	A	20000430	MX 1999-12090		19991217	<--
HK 1024686	A1	20030321	HK 2000-102386		20000420	<--
PRIORITY APPLN. INFO.:			US 1997-877739	A	19970617	<--
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OTHER SOURCE(S): MARPAT 130:81410
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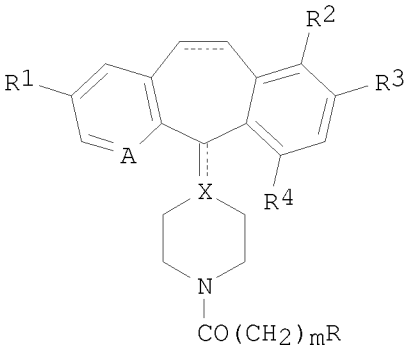

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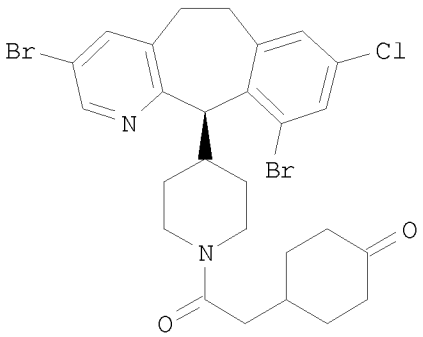


II

AB Title compds. (I; A = N, NO; R1, R3 = halo; R2, R4 = H, halo provided that ≥1 = H; X = C, CH, N; R = substituted cycloalkyl, heterocycloalkyl; dotted lines = optional double bonds; m = 0-2; R = substituted cyclobutyl(idene), cyclopentyl(idene), cyclohexyl(idene), indanyl(idene),

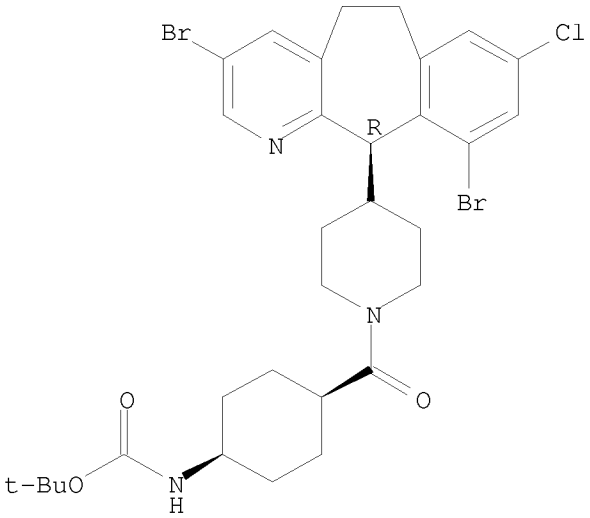
azetidinyl, piperidinyl, etc.), were prepared Thus, tested I including title compound (II) inhibited farnesyl protein transferase with IC50's in the range 1.9 nM to >160 nM.

IT 218772-00-0P 218772-01-1P 218772-02-2P
218772-03-3P 218772-08-8P 218772-09-9P
218772-10-2P 218772-11-3P 218772-14-6P
218772-15-7P 218772-16-8P 218772-17-9P
218772-27-1P 218772-28-2P 218772-29-3P
218772-30-6P 218772-31-7P 218772-35-1P
218772-36-2P 218772-37-3P 218772-93-1P
218772-94-2P 218772-95-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 11-piperidinylbenzo[5,6]cyclohepta[1,2-b]pyridines and related compds. as inhibitors of farnesyl protein transferase)

RN 218772-00-0 CAPLUS

CN Carbamic acid, [cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

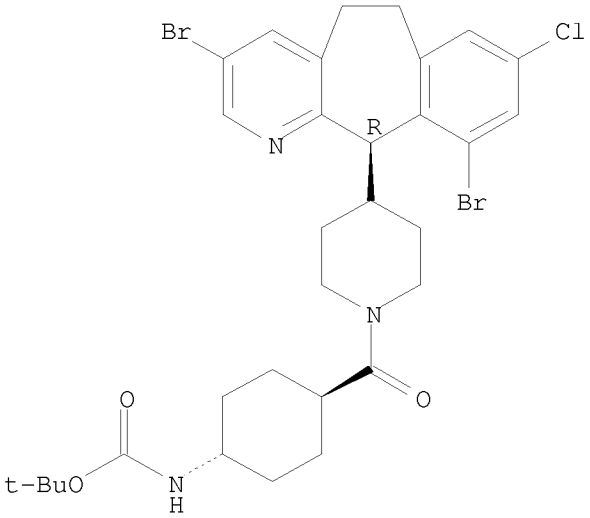
Absolute stereochemistry.



RN 218772-01-1 CAPLUS

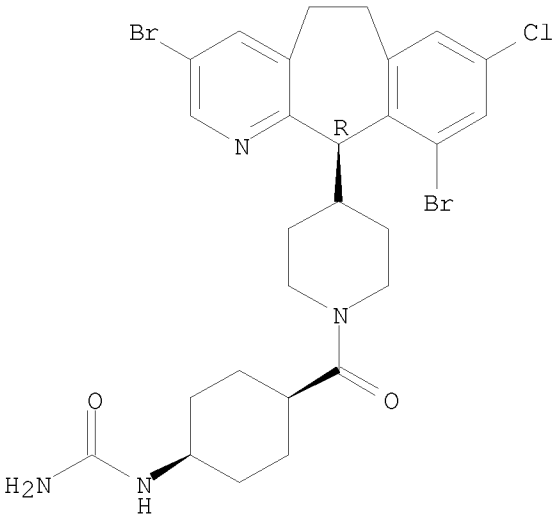
CN Carbamic acid, [trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



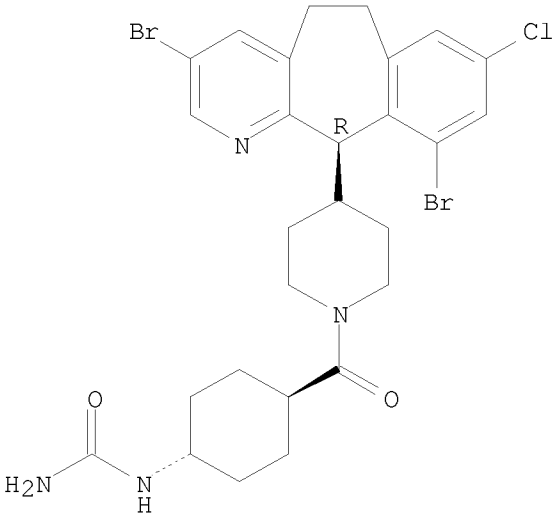
RN 218772-02-2 CAPLUS
CN Urea, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



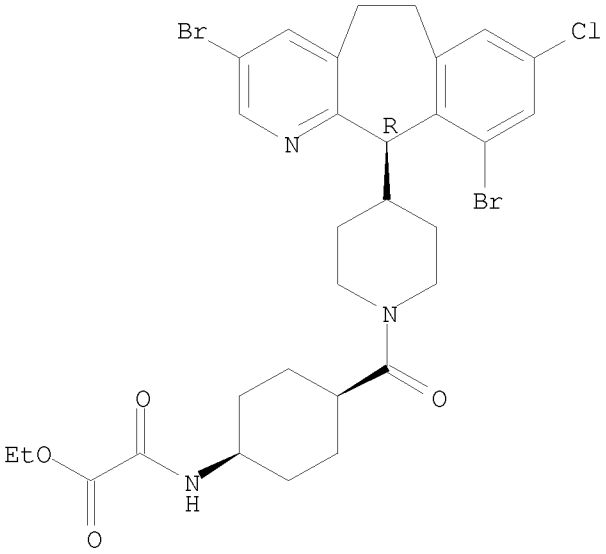
RN 218772-03-3 CAPLUS
CN Urea, N-[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



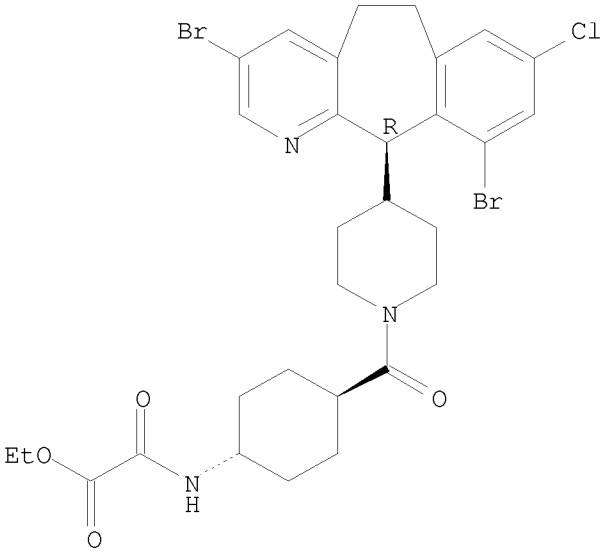
RN 218772-08-8 CAPLUS
CN Acetic acid, 2-[[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



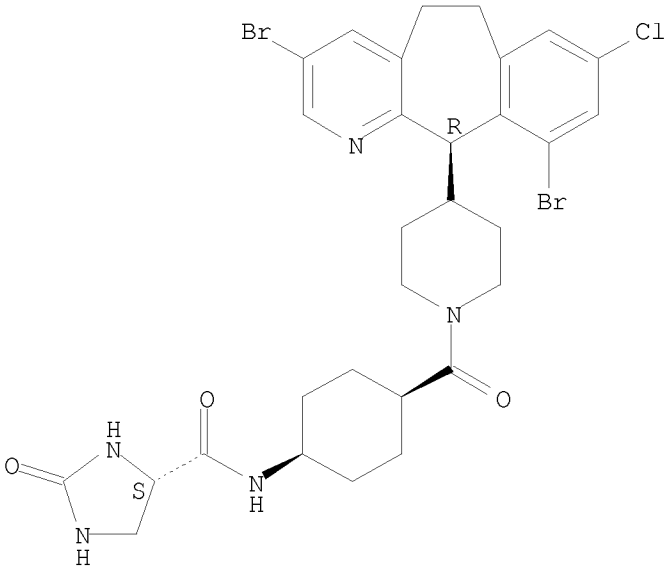
RN 218772-09-9 CAPLUS
CN Acetic acid, 2-[[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 218772-10-2 CAPLUS
CN 4-Imidazolidinecarboxamide, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

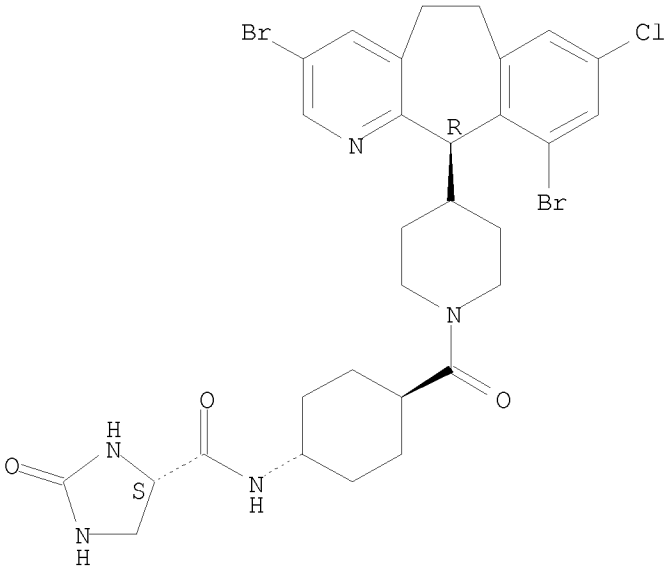
Absolute stereochemistry.



RN 218772-11-3 CAPLUS

CN 4-Imidazolidinecarboxamide, N-[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

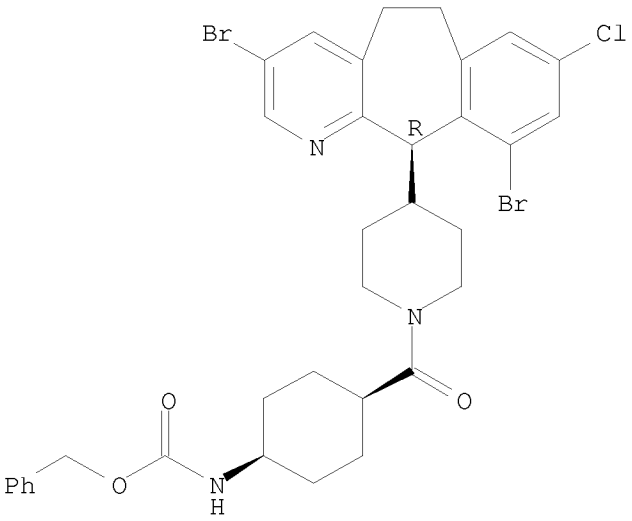
Absolute stereochemistry.



RN 218772-14-6 CAPLUS

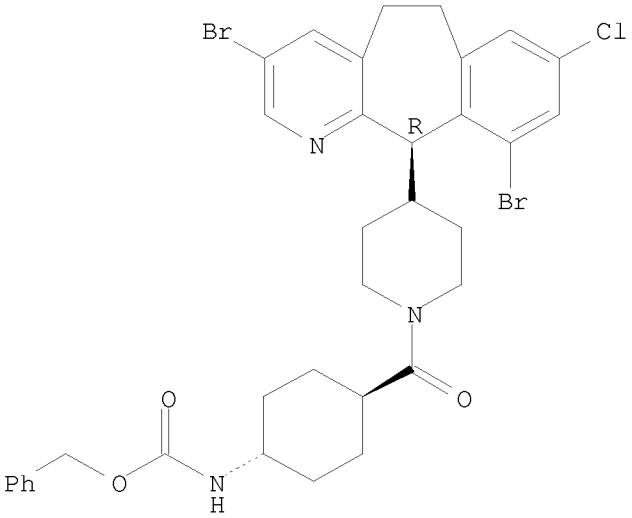
CN Carbamic acid, [cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



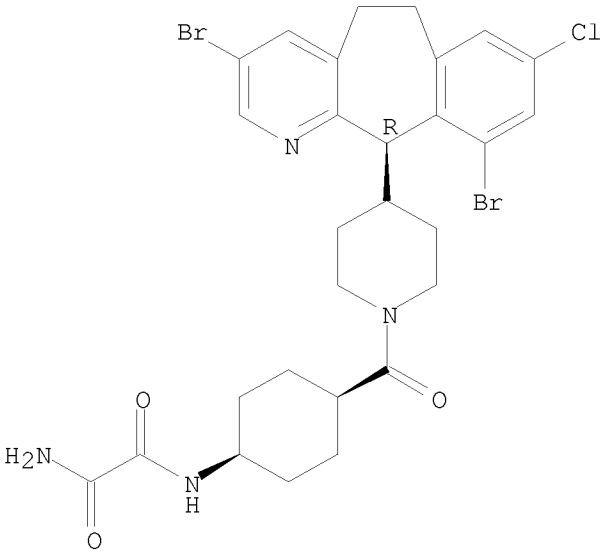
RN 218772-15-7 CAPLUS
CN Carbamic acid, [trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



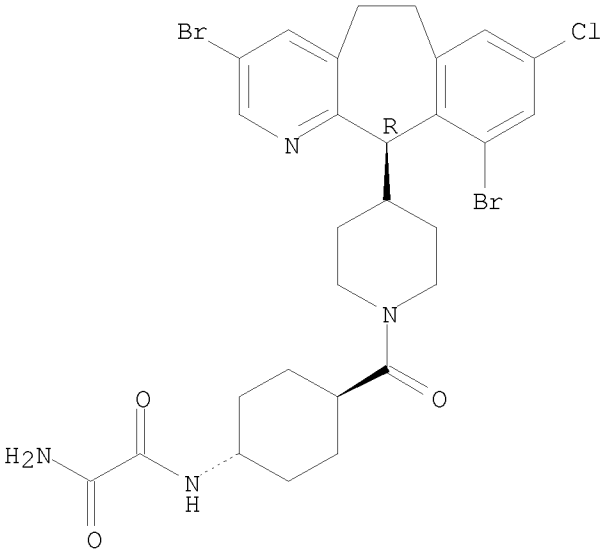
RN 218772-16-8 CAPLUS
CN Ethanediamide, N1-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



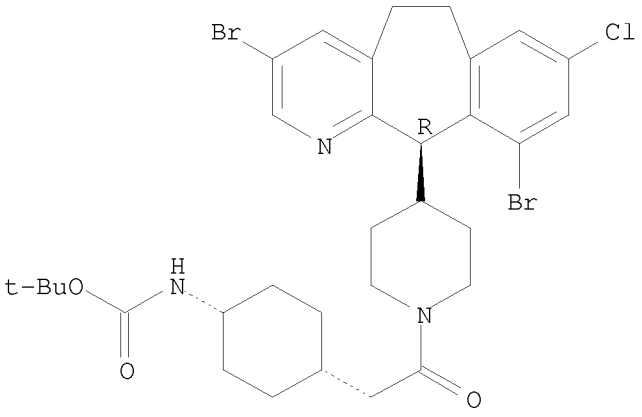
RN 218772-17-9 CAPLUS
CN Ethanediamide, N1-[trans-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 218772-27-1 CAPLUS
CN Carbamic acid, [cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

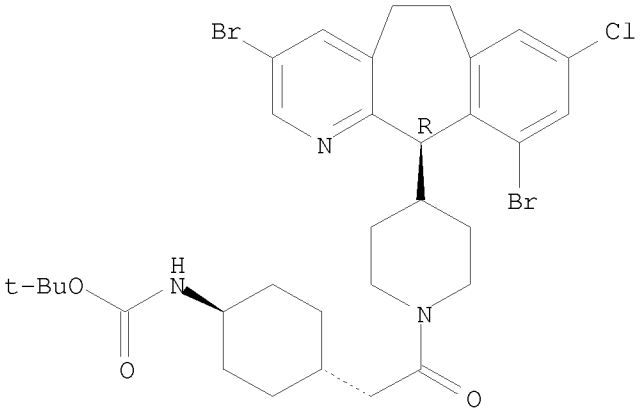
Absolute stereochemistry.



RN 218772-28-2 CAPLUS

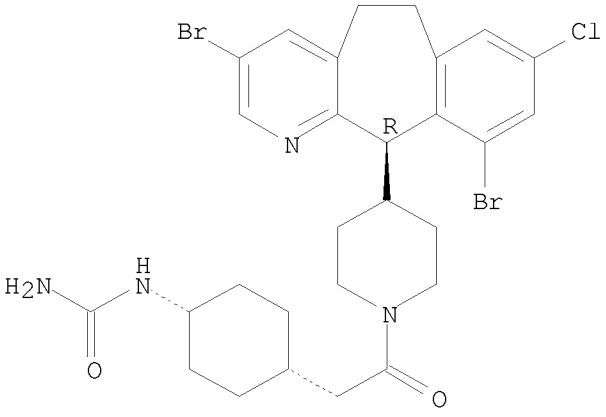
CN Carbamic acid, [trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



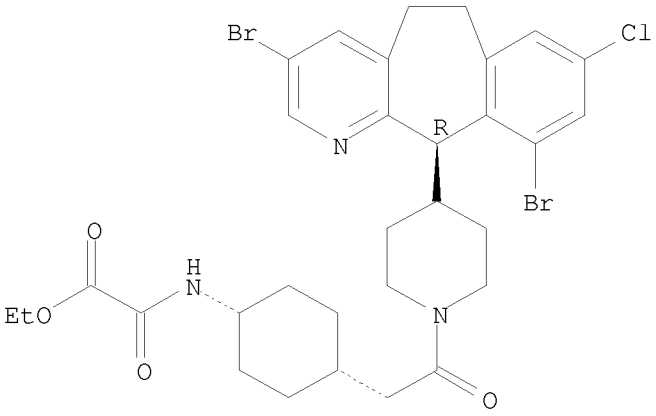
RN 218772-29-3 CAPLUS
CN Urea, N-[cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



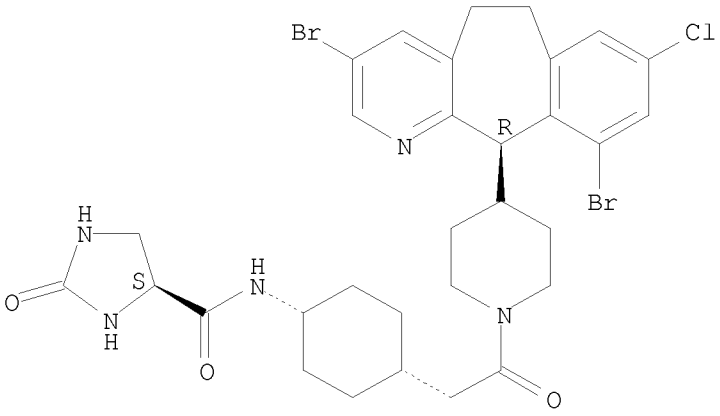
RN 218772-30-6 CAPLUS
CN Acetic acid, 2-[[cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



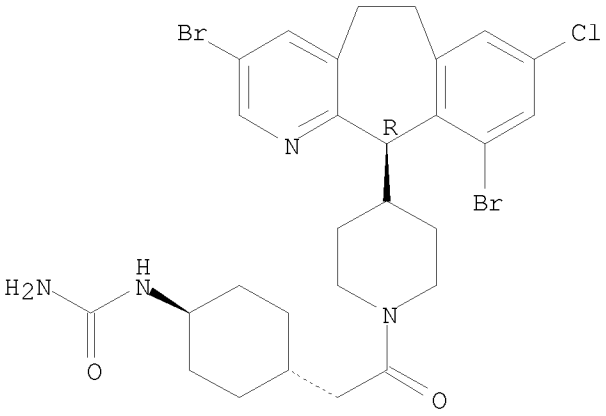
RN 218772-31-7 CAPLUS
CN 4-Imidazolidinecarboxamide, N-[cis-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



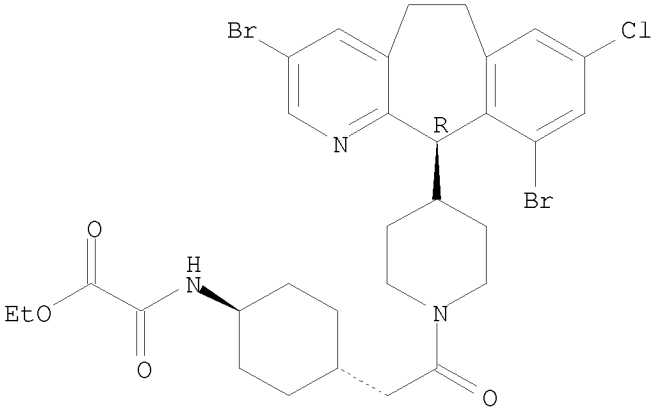
RN 218772-35-1 CAPLUS
CN Urea, N-[trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



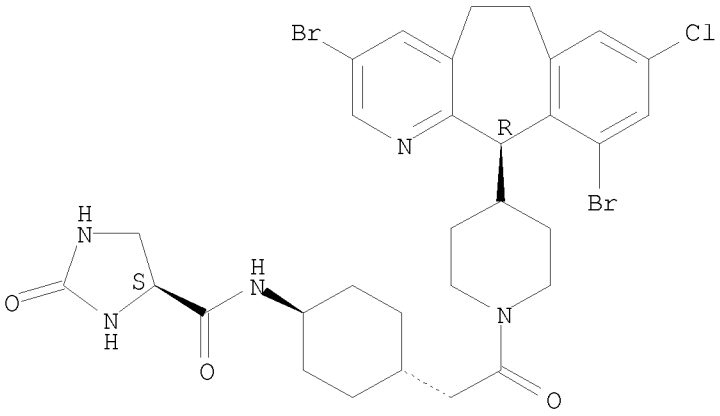
RN 218772-36-2 CAPLUS
CN Acetic acid, 2-[[trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]amino]-2-oxo-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



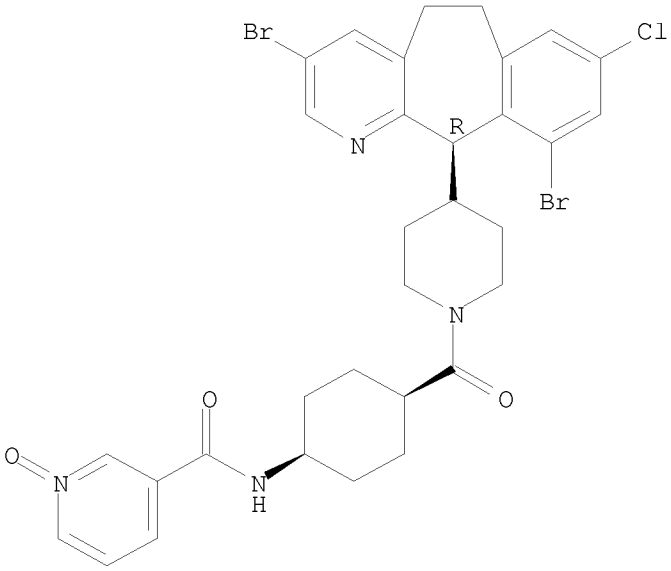
RN 218772-37-3 CAPLUS
CN 4-Imidazolidinecarboxamide, N-[trans-4-[2-[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]-2-oxoethyl]cyclohexyl]-2-oxo-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



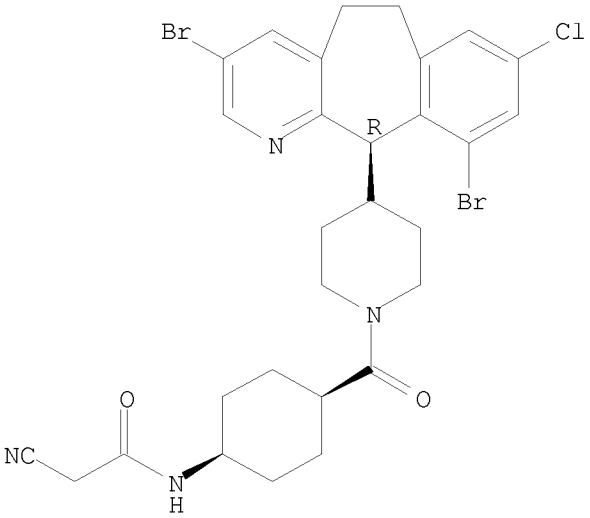
RN 218772-93-1 CAPLUS
CN 3-Pyridinecarboxamide, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]-, 1-oxide (CA INDEX NAME)

Absolute stereochemistry.



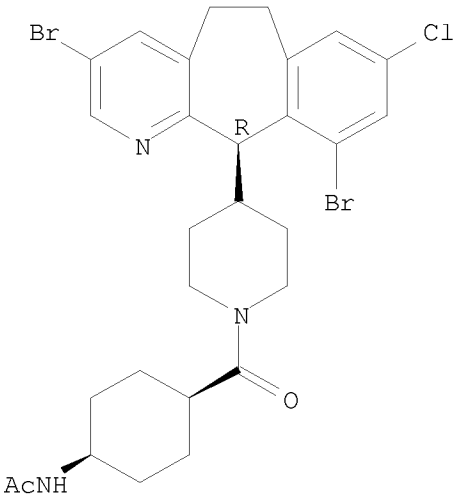
RN 218772-94-2 CAPLUS
CN Acetamide, 2-cyano-N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 218772-95-3 CAPLUS
CN Acetamide, N-[cis-4-[[4-[(11R)-3,10-dibromo-8-chloro-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-yl]-1-piperidinyl]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

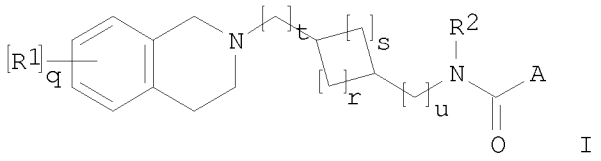
L18 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:761882 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 130:13926
TITLE: Preparation of substituted tetrahydroisoquinoline derivatives as modulators of dopamine D3 receptors

INVENTOR(S): Johnson, Christopher Norbert; Stemp, Geoffrey
PATENT ASSIGNEE(S): Smithkline Beecham PLC, UK
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

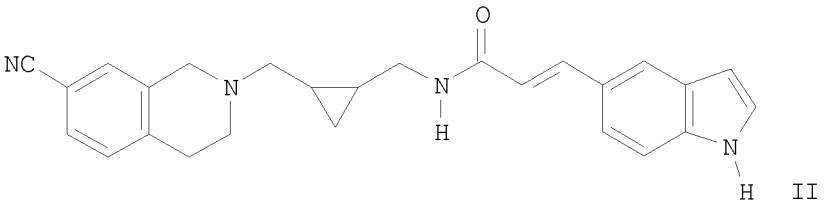
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9851671	A1	19981119	WO 1998-EP2584	19980428 <--
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2288850	A1	19981119	CA 1998-2288850	19980428 <--
EP 983245	A1	20000308	EP 1998-924263	19980428 <--
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2001525813	T	20011211	JP 1998-548741	19980428 <--

PRIORITY APPLN. INFO.: GB 1997-9303 A 19970509 <--
WO 1998-EP2584 W 19980428 <--

OTHER SOURCE(S): MARPAT 130:13926
GI



I



II

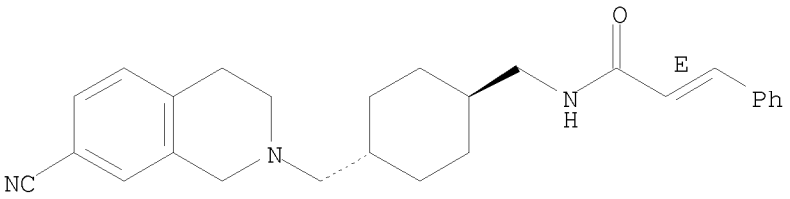
AB The title compds. [I; R1 = H, halo, OH, etc.; s = 0-2; r = 1-4 (such that the sum of s + r = 1-4; t = 0-1; u = 0-2; R2 = H, C1-4 alkyl; q = 1-2; A = Ar, Ar1YAr2, (E)-CH:CH-Ar wherein Ar = (un)substituted Ph, 5-6 membered aromatic heterocyclic ring, bicyclic ring; Ar1, Ar2 = (un)substituted Ph, 5-6 membered aromatic heterocyclic ring; Y = a bond, NHCO, CONH, etc.)] which have affinity for dopamine receptors, in particular the D3 receptor, and thus are potentially useful in the treatment of conditions wherein modulation of the D3 receptor is beneficial, e.g. as antipsychotic agents,

were prepared and formulated. Thus, reaction of (±)-trans-1-aminomethyl-2-[2-(7-cyano-1,2,3,4-tetrahydro)isoquinolyl]methylcyclopropane (preparation described) with (E)-3-(5-indolyl)propenoic acid afforded 66% the title compound trans-(E)-II. Prepared compds. I showed pKi of 7.0-8.5 at the human cloned dopamine D3 receptor.

IT 216144-10-4P 216144-19-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted tetrahydroisoquinoline derivs. as modulators of dopamine D3 receptors)

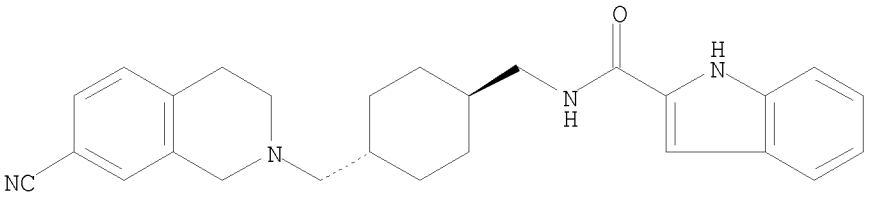
RN 216144-10-4 CAPLUS
CN 2-Propenamide, N-[[trans-4-[(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)methyl]cyclohexyl]methyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 216144-19-3 CAPLUS
CN 1H-Indole-2-carboxamide, N-[[trans-4-[(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)methyl]cyclohexyl]methyl]- (CA INDEX NAME)

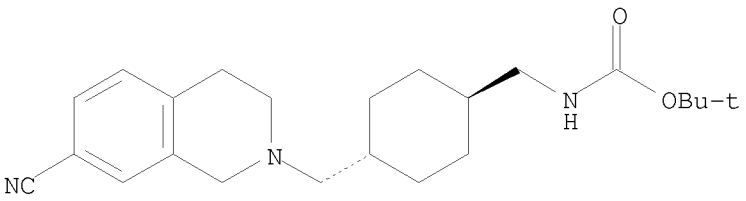
Relative stereochemistry.



IT 216144-33-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted tetrahydroisoquinoline derivs. as modulators of dopamine D3 receptors)

RN 216144-33-1 CAPLUS
CN Carbamic acid, [[trans-4-[(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:745036 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 130:3775
TITLE: Preparation of N-[2-(4-carboxamidocyclohexyl)ethyl]tetrahydroisoquinolines as dopamine D3 receptor ligands
INVENTOR(S): Branch, Clive Leslie; Johnson, Christopher Norbert; Stemp, Geoffrey
PATENT ASSIGNEE(S): Smithkline Beecham PLC, UK
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9850364	A1	19981112	WO 1998-EP2583	19980427 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2288899	A1	19981112	CA 1998-2288899	19980427 <--
AU 9876518	A	19981127	AU 1998-76518	19980427 <--
AU 725491	B2	20001012		
EP 983244	A1	20000308	EP 1998-924262	19980427 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI				
TR 9902724	T2	20000421	TR 1999-2724	19980427 <--
HU 2000003608	A2	20010328	HU 2000-3608	19980427 <--
HU 2000003608	A3	20010628		
BR 9809591	A	20010911	BR 1998-9591	19980427 <--
JP 2002501506	T	20020115	JP 1998-547712	19980427 <--
ZA 9803659	A	19991101	ZA 1998-3659	19980430 <--
NO 9905338	A	19991102	NO 1999-5338	19991102 <--
MX 9910101	A	20000430	MX 1999-10101	19991103 <--

US 6465485 B1 20021015 US 2000-656379 20000906 <--
PRIORITY APPLN. INFO.: GB 1997-8976 A 19970503 <--
GB 1997-23294 A 19971104 <--
WO 1998-EP2583 W 19980427 <--
US 1999-423163 B1 19991102 <--

OTHER SOURCE(S): MARPAT 130:3775

AB R1CH2CH2ZNR2COR (Z = 1,4-cyclohexylene)[I; R = (un)substituted Ph, -heteroaryl, (E)-CH:CHPh, etc.; R1 = benzene ring-(un)substituted 1,2,3,4-tetrahydroisoquinolin-2-yl; R2 = H or alkyl] were prepared Thus, 8-(2-hydroxyethyl)-1,4-dioxaspiro[4.5]decane was oxidized and the product reductively aminated by 7-cyano-1,2,3,4-tetrahydroisoquinoline to give, after deprotection and reductive amination, cis- and trans-2-[2-(4-aminocyclohexyl)ethyl]-7-cyano-1,2,3,4-tetrahydroisoquinoline. The latter mixture was treated with indole-2-carboxylic acid under amidation conditions to give trans-I (R = 2-indolyl, R1 = 7-cyano-1,2,3,4-tetrahydroisoquinolin-2-yl, R2 = H). Data for biol. activity of I were given.

IT 215802-15-6P 215802-16-7P 215802-17-8P
215802-18-9P 215802-20-3P 215802-21-4P
215802-22-5P 215802-23-6P 215802-24-7P
215802-25-8P 215802-26-9P 215802-27-0P
215802-29-2P 215802-32-7P 215802-34-9P
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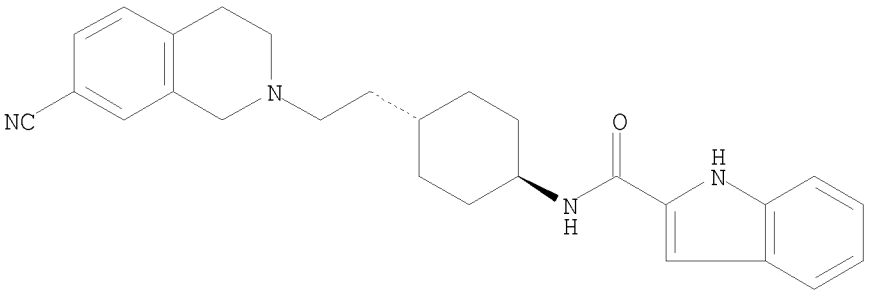
215804-56-1P 215804-57-2P 215804-58-3P
215804-60-7P 215804-61-8P 215804-62-9P
215804-66-3P 215804-67-4P 215805-72-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-{2-(4-carboxamidocyclohexyl)ethyl]tetrahydroisoquinolines as dopamine D3 receptor ligands)

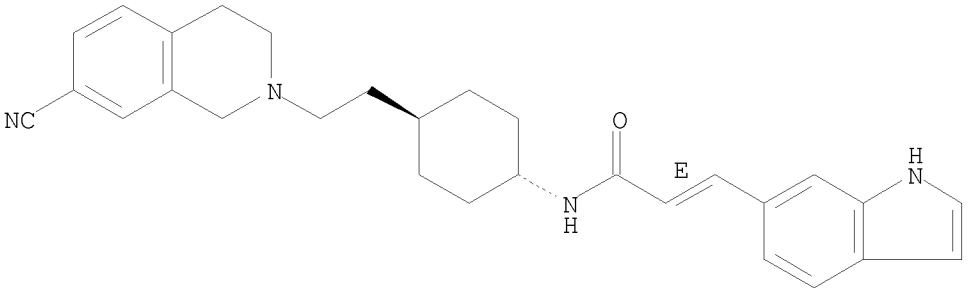
RN 215802-15-6 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



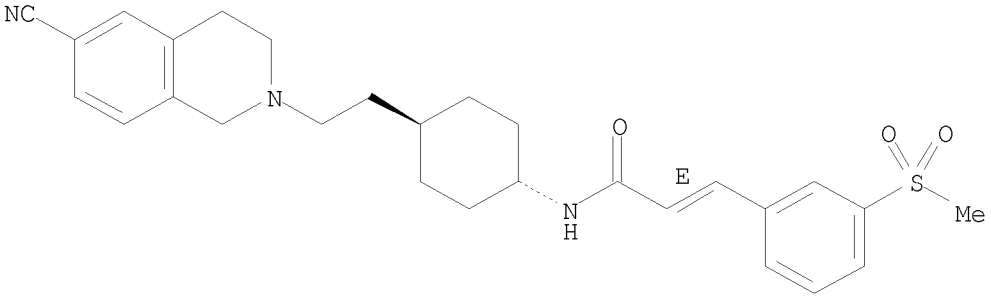
RN 215802-16-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(1H-indol-6-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



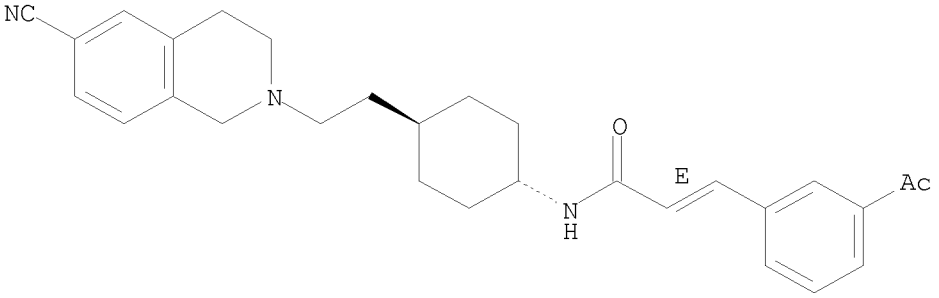
RN 215802-17-8 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[3-(methylsulfonyl)phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



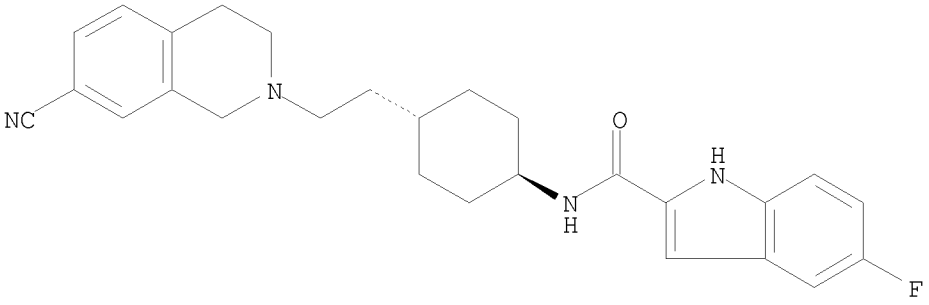
RN 215802-18-9 CAPLUS
CN 2-Propenamide, 3-(3-acetylphenyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



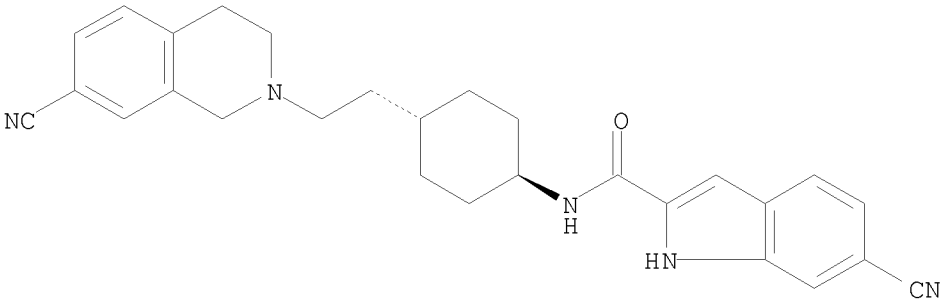
RN 215802-20-3 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-fluoro- (CA INDEX NAME)

Relative stereochemistry.



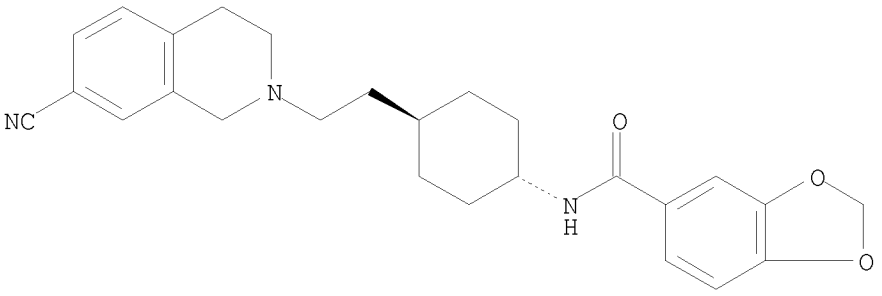
RN 215802-21-4 CAPLUS
CN 1H-Indole-2-carboxamide, 6-cyano-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



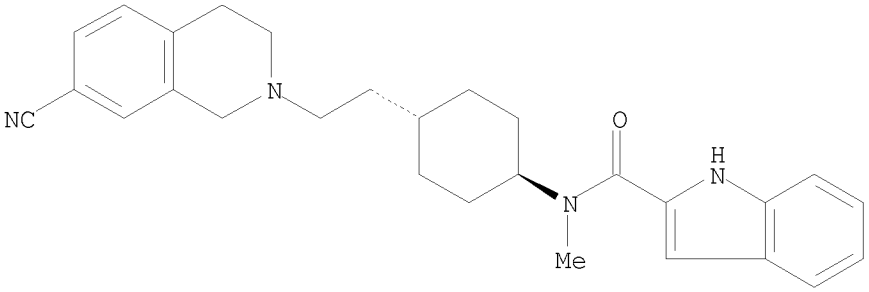
RN 215802-22-5 CAPLUS
CN 1,3-Benzodioxole-5-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



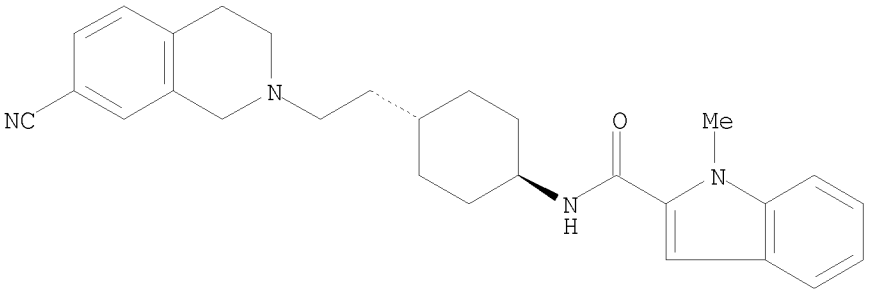
RN 215802-23-6 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.



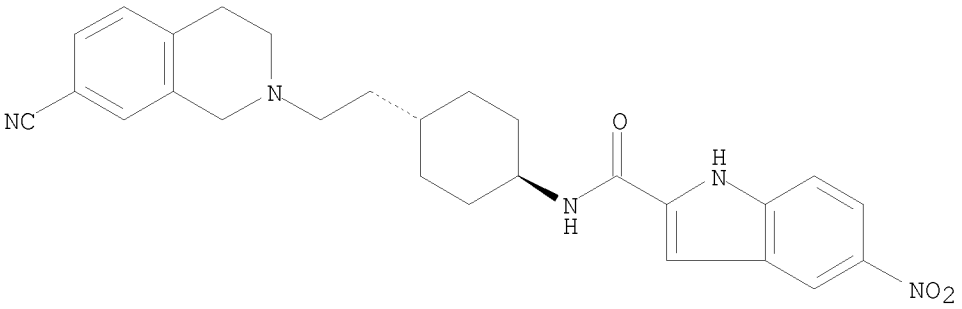
RN 215802-24-7 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-1-methyl- (CA INDEX NAME)

Relative stereochemistry.



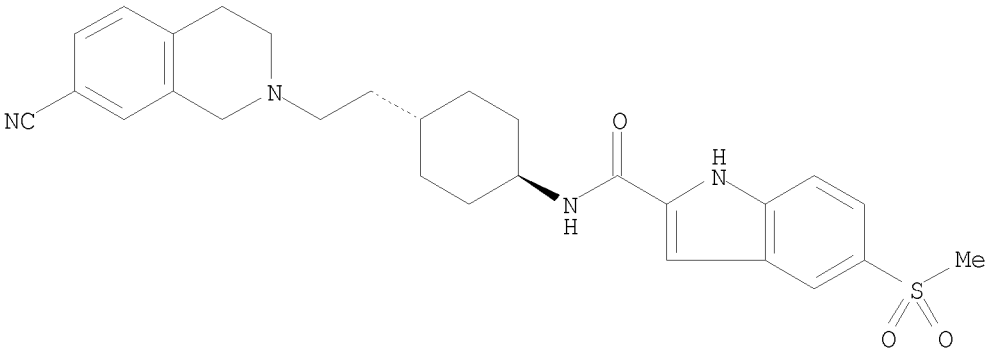
RN 215802-25-8 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-nitro- (CA INDEX NAME)

Relative stereochemistry.



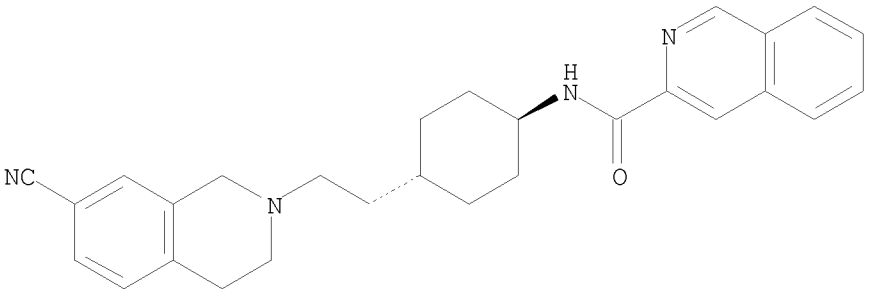
RN 215802-26-9 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-(methylsulfonyl)- (CA INDEX NAME)

Relative stereochemistry.



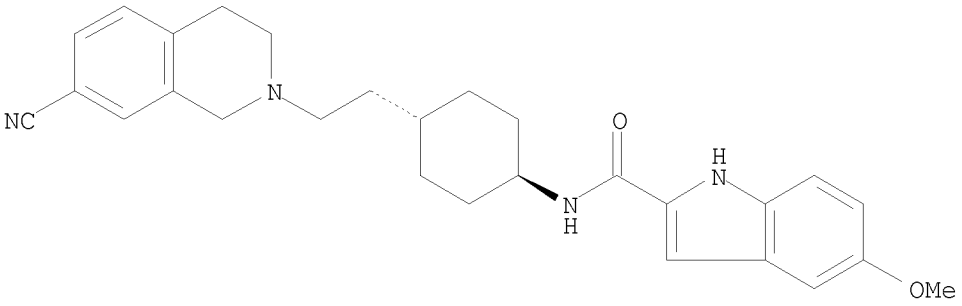
RN 215802-27-0 CAPLUS
CN 3-Isoquinolinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



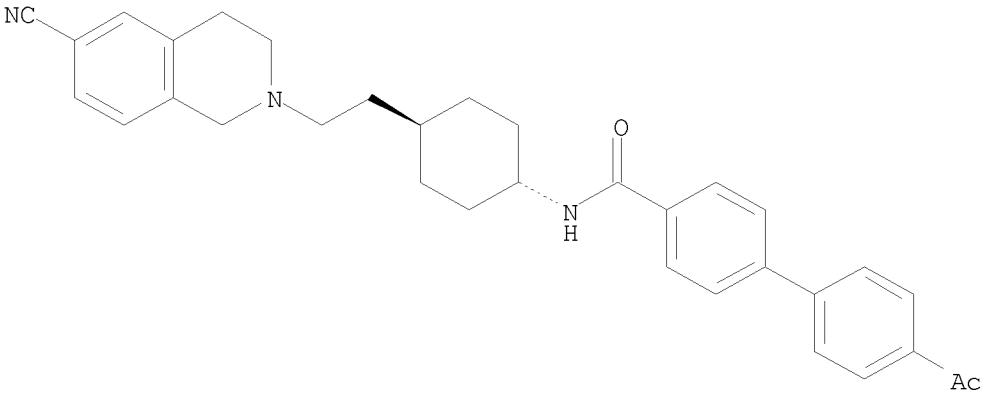
RN 215802-29-2 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-methoxy- (CA INDEX NAME)

Relative stereochemistry.



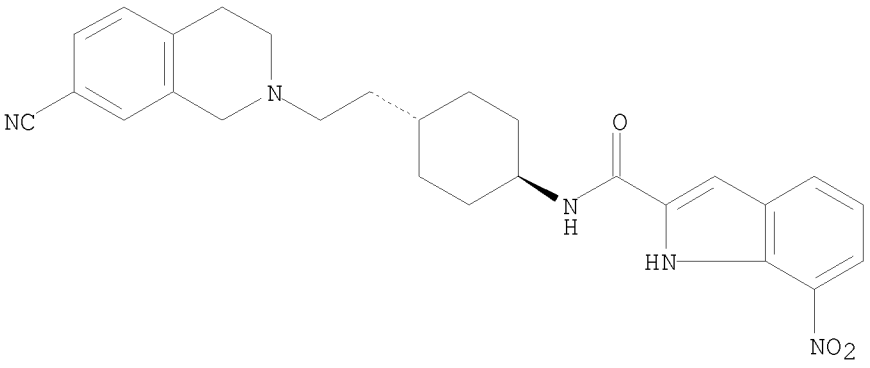
RN 215802-32-7 CAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, 4'-acetyl-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



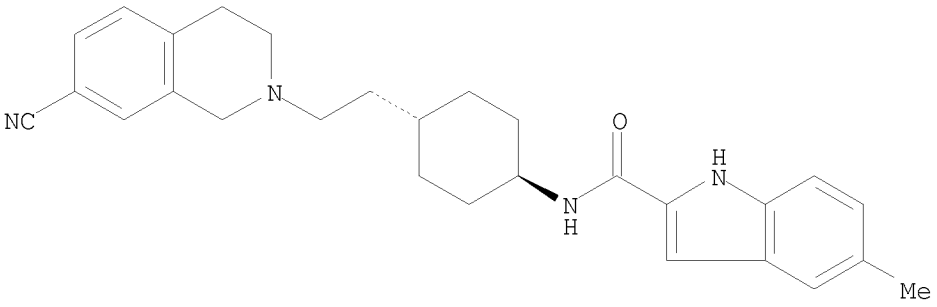
RN 215802-34-9 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-7-nitro- (CA INDEX NAME)

Relative stereochemistry.



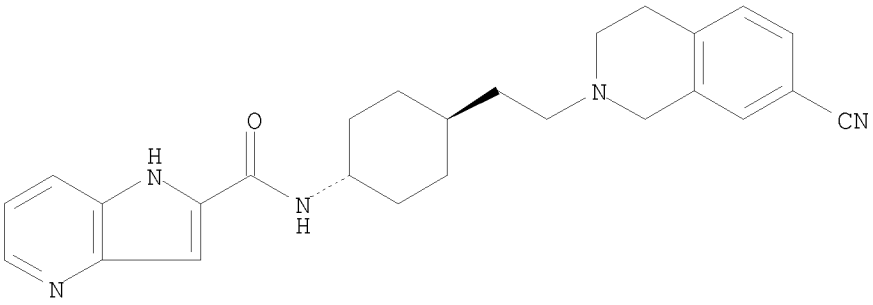
RN 215802-36-1 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-methyl- (CA INDEX NAME)

Relative stereochemistry.



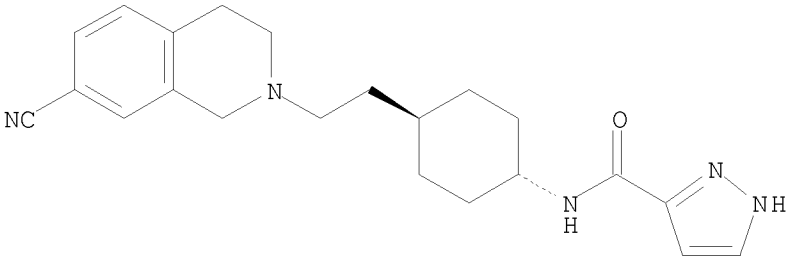
RN 215802-38-3 CAPLUS
CN 1H-Pyrrolo[3,2-b]pyridine-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



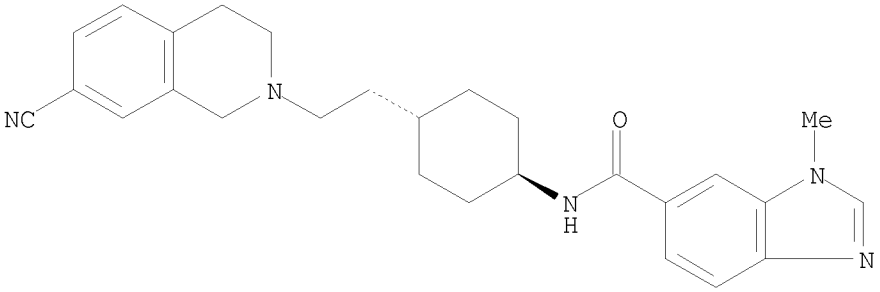
RN 215802-41-8 CAPLUS
CN 1H-Pyrazole-3-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



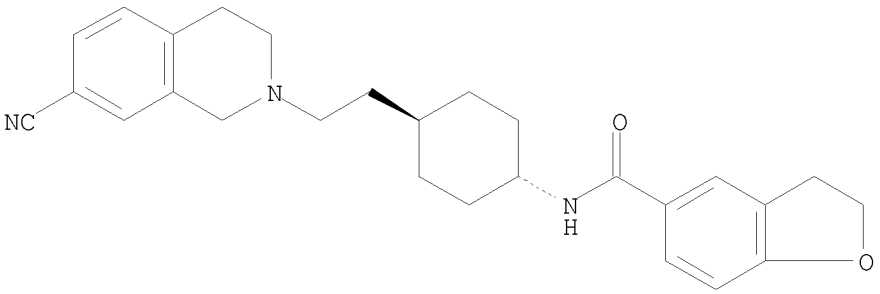
RN 215802-43-0 CAPLUS
CN 1H-Benzimidazole-6-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-1-methyl- (CA INDEX NAME)

Relative stereochemistry.



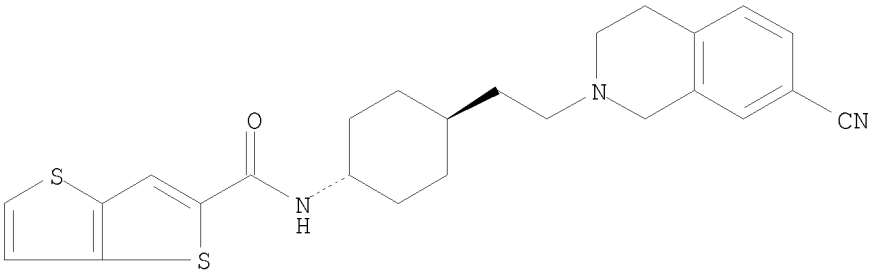
RN 215802-45-2 CAPLUS
CN 5-Benzofurancarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2,3-dihydro- (CA INDEX NAME)

Relative stereochemistry.



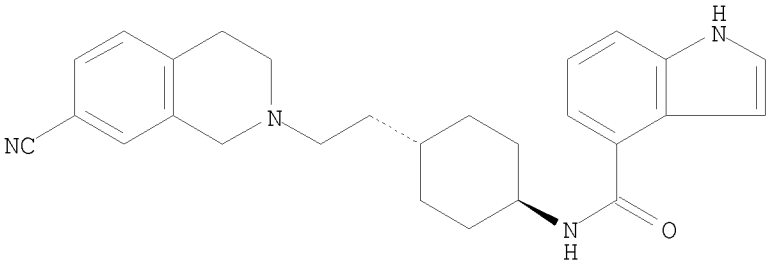
RN 215802-47-4 CAPLUS
CN Thieno[3,2-b]thiophene-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



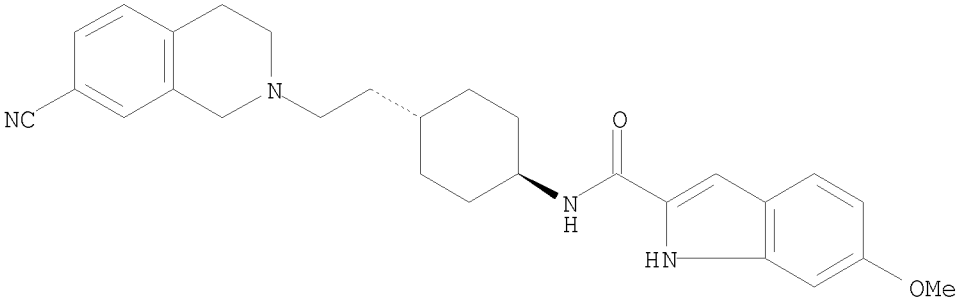
RN 215802-49-6 CAPLUS
CN 1H-Indole-4-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



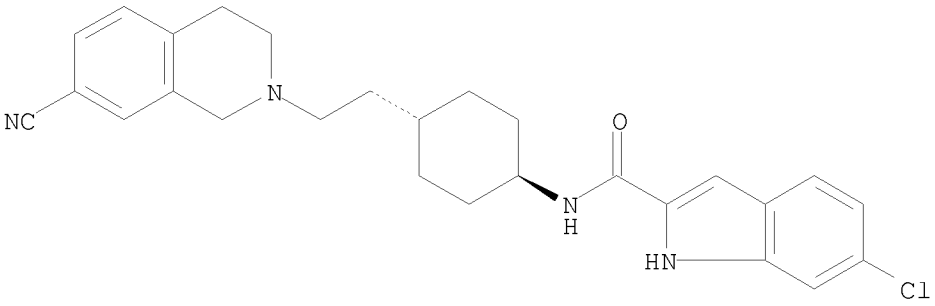
RN 215802-51-0 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-methoxy- (CA INDEX NAME)

Relative stereochemistry.



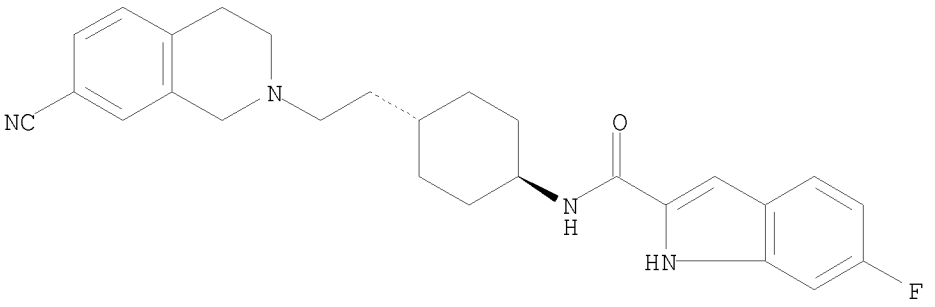
RN 215802-54-3 CAPLUS
CN 1H-Indole-2-carboxamide, 6-chloro-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



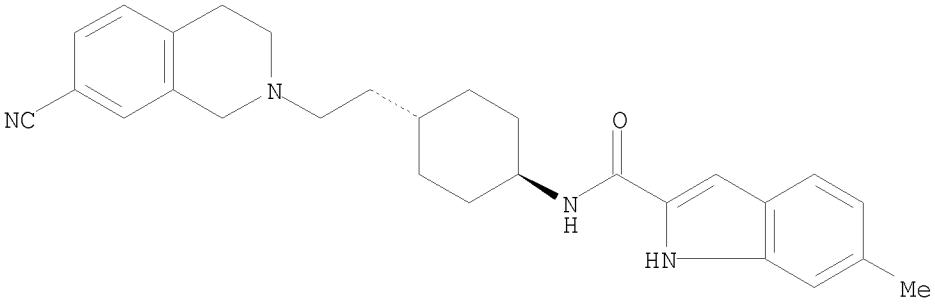
RN 215802-56-5 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-fluoro- (CA INDEX NAME)

Relative stereochemistry.



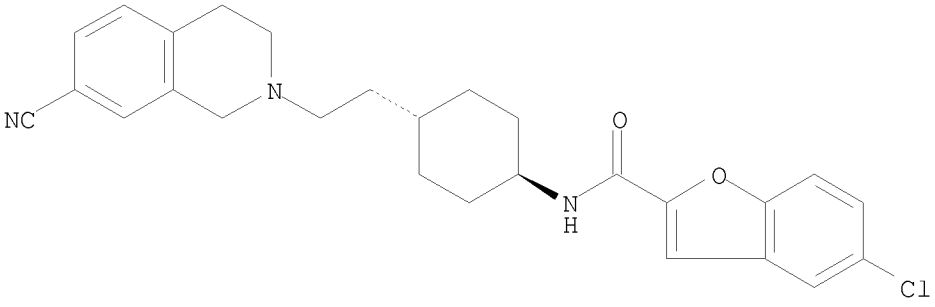
RN 215802-58-7 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-methyl- (CA INDEX NAME)

Relative stereochemistry.



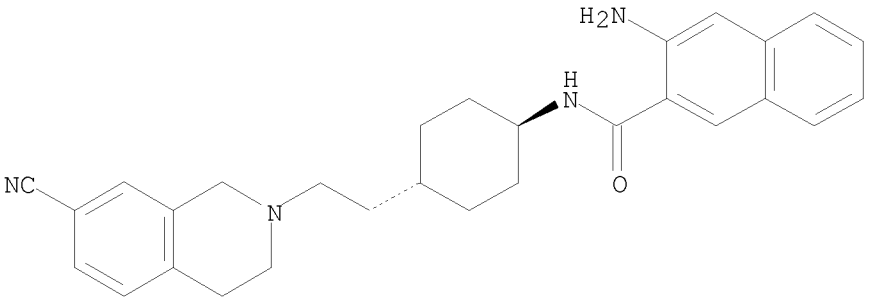
RN 215802-60-1 CAPLUS
CN 2-Benzofurancarboxamide, 5-chloro-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



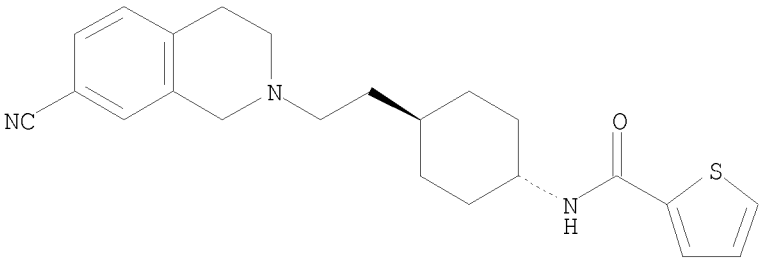
RN 215802-62-3 CAPLUS
CN 2-Naphthalenecarboxamide, 3-amino-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



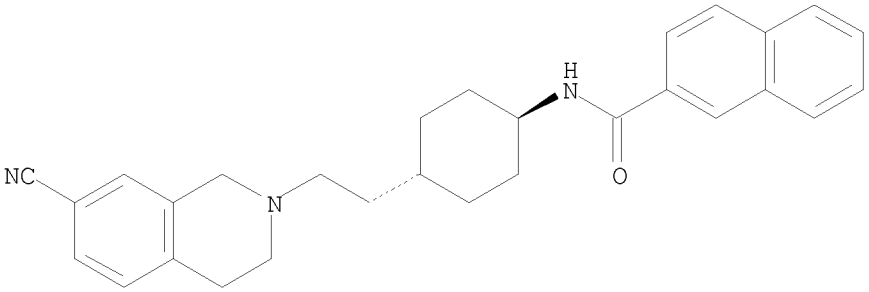
RN 215802-64-5 CAPLUS
CN 2-Thiophenecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



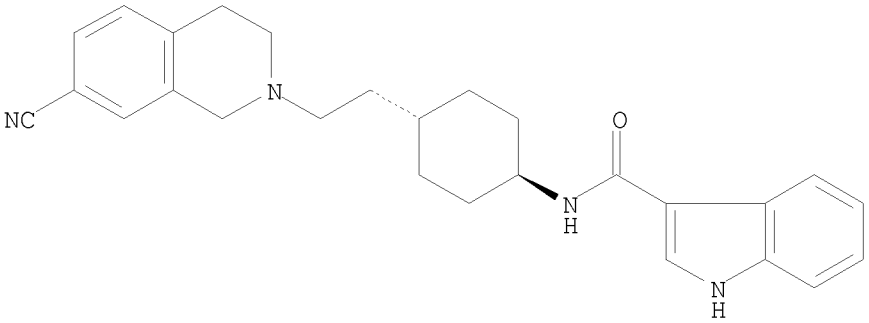
RN 215802-66-7 CAPLUS
CN 2-Naphthalenecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



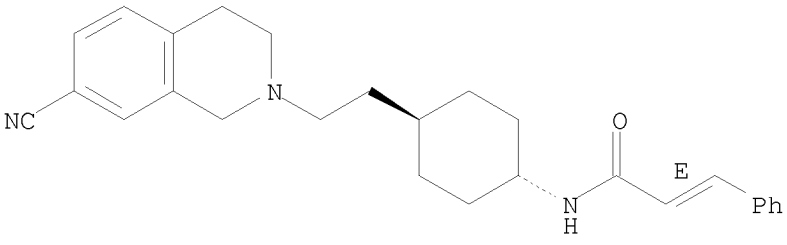
RN 215802-69-0 CAPLUS
CN 1H-Indole-3-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



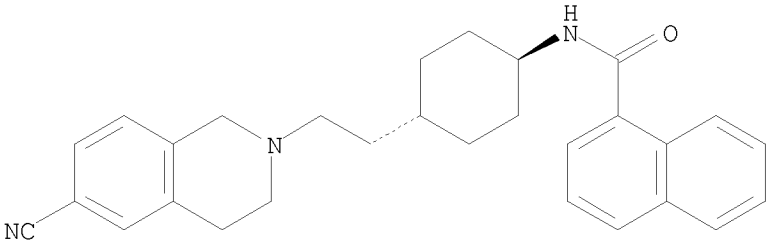
RN 215802-71-4 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



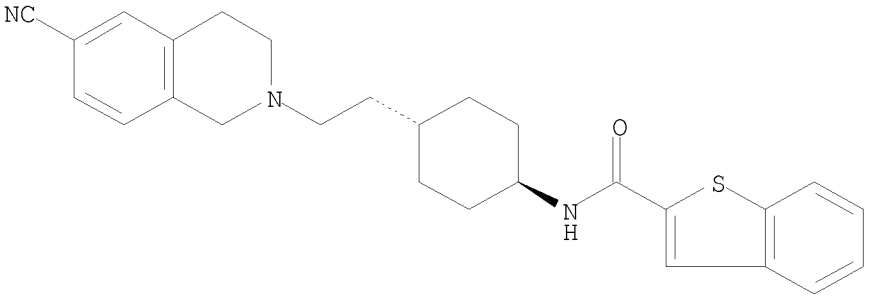
RN 215802-73-6 CAPLUS
CN 1-Naphthalenecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



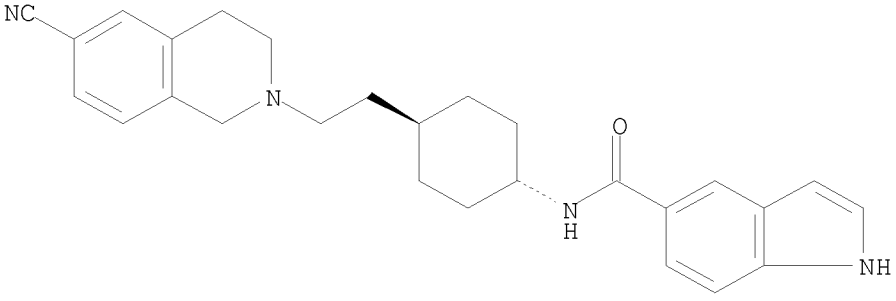
RN 215802-75-8 CAPLUS
CN Benzo[b]thiophene-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



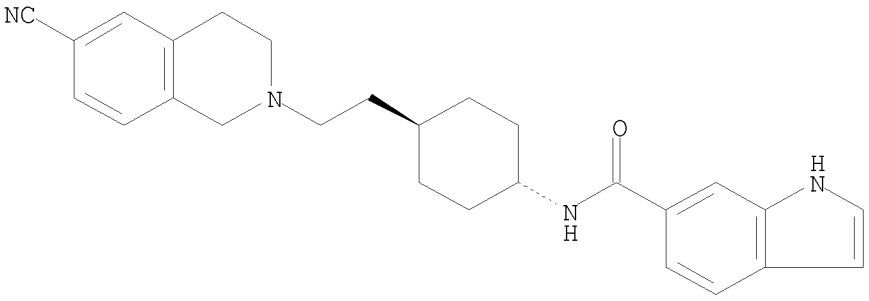
RN 215802-78-1 CAPLUS
CN 1H-Indole-5-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



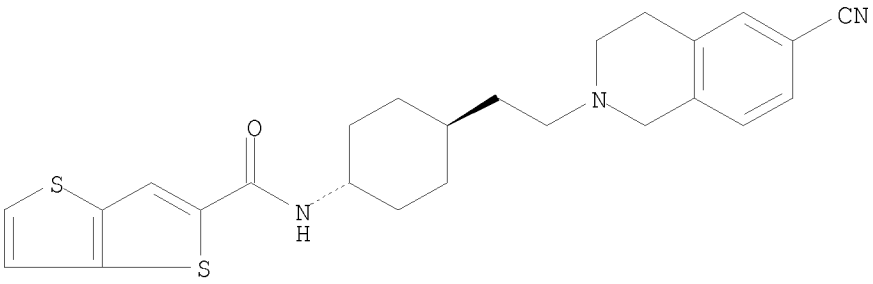
RN 215802-80-5 CAPLUS
CN 1H-Indole-6-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



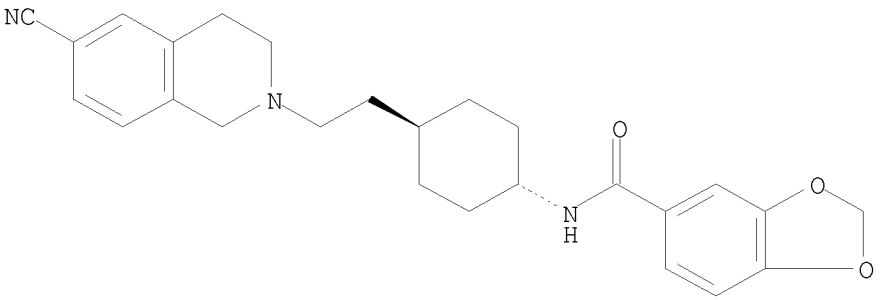
RN 215802-81-6 CAPLUS
CN Thieno[3,2-b]thiophene-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



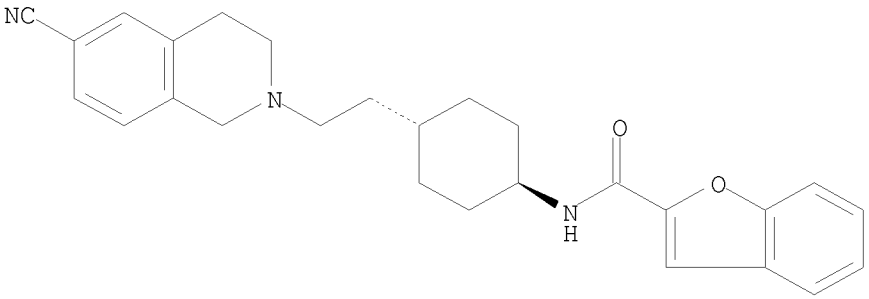
RN 215802-82-7 CAPLUS
CN 1,3-Benzodioxole-5-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



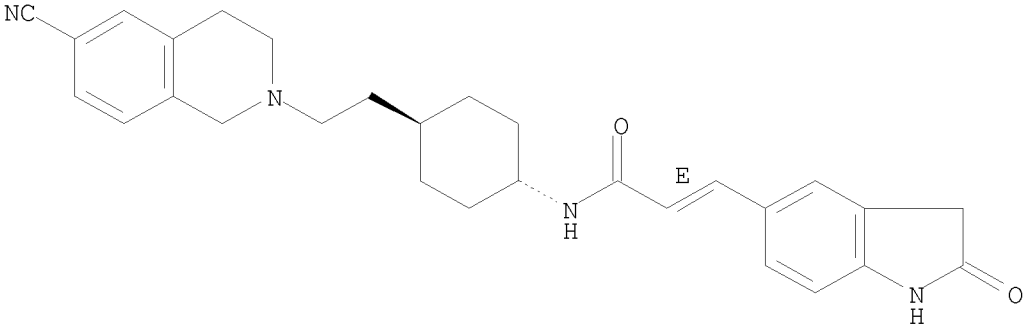
RN 215802-83-8 CAPLUS
CN 2-Benzofurancarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



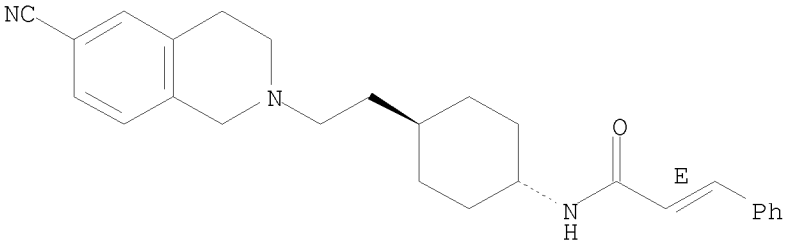
RN 215802-85-0 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2,3-dihydro-2-oxo-1H-indol-5-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



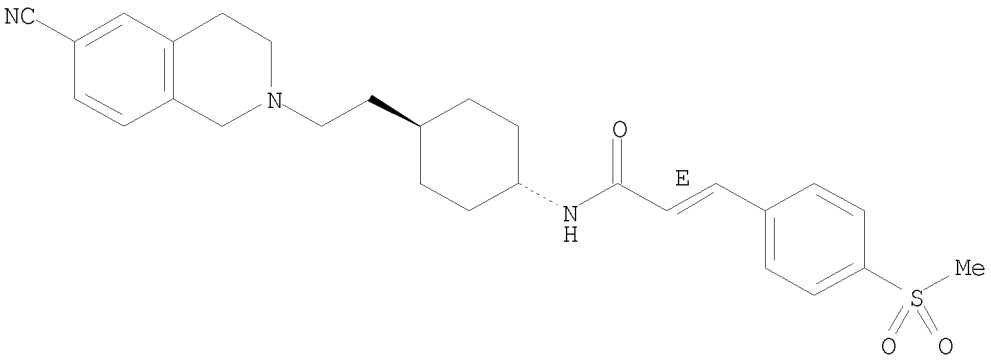
RN 215802-86-1 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



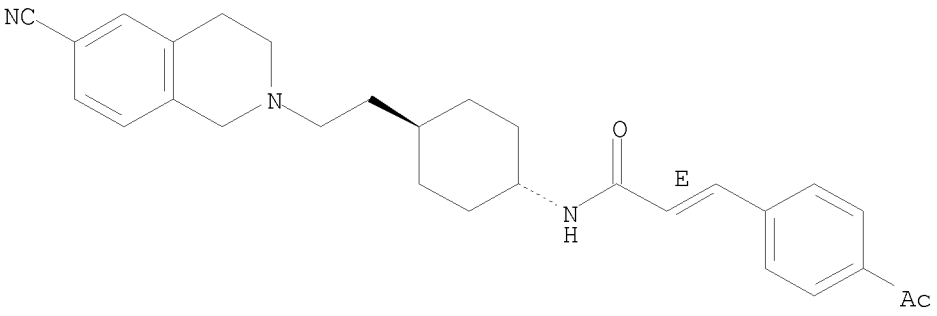
RN 215802-87-2 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[4-(methylsulfonyl)phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



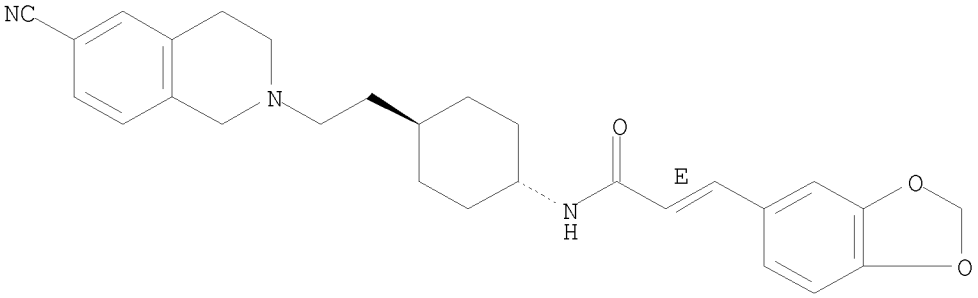
RN 215802-88-3 CAPLUS
CN 2-Propenamide, 3-(4-acetylphenyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



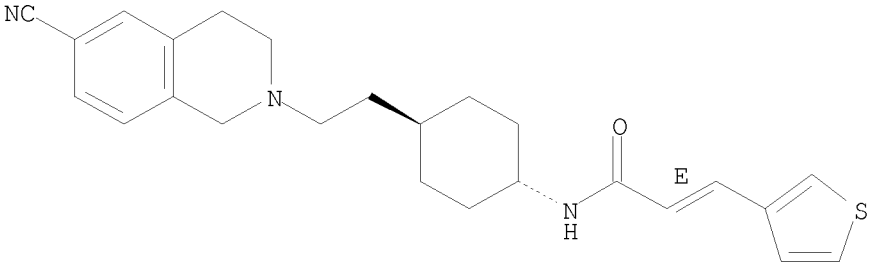
RN 215802-89-4 CAPLUS
CN 2-Propenamide, 3-(1,3-benzodioxol-5-yl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 215802-90-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3-thienyl)-, (2E)- (CA INDEX NAME)

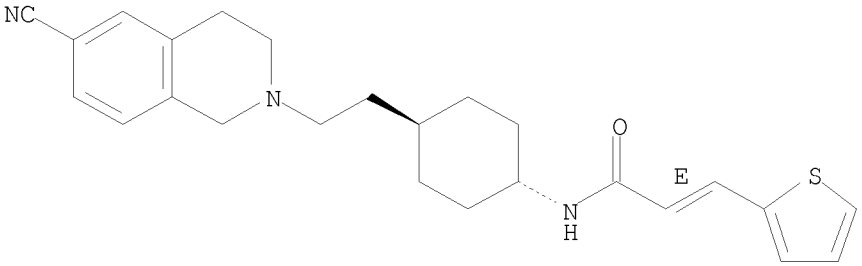
Relative stereochemistry.
Double bond geometry as shown.



RN 215802-91-8 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-

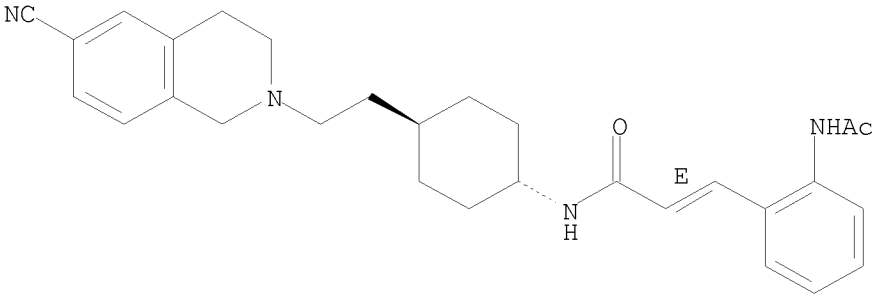
isoquinolinyl)ethyl]cyclohexyl]-3-(2-thienyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



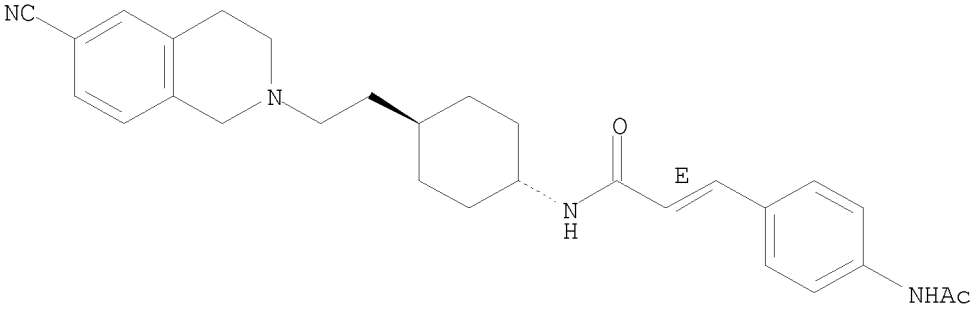
RN 215802-92-9 CAPLUS
CN 2-Propenamide, 3-[2-(acetylamino)phenyl]-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



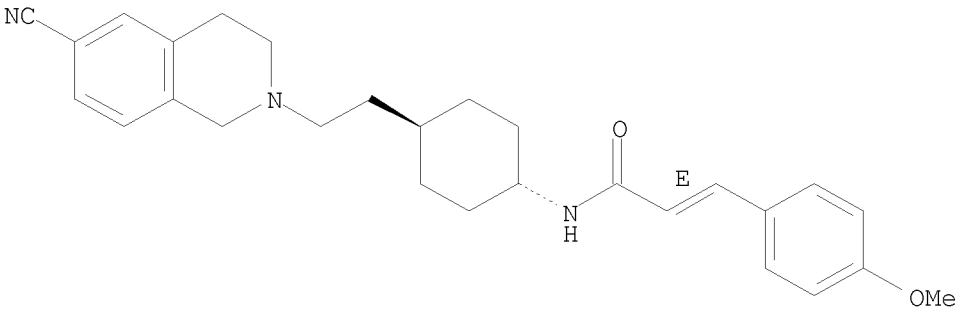
RN 215802-93-0 CAPLUS
CN 2-Propenamide, 3-[4-(acetylamino)phenyl]-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



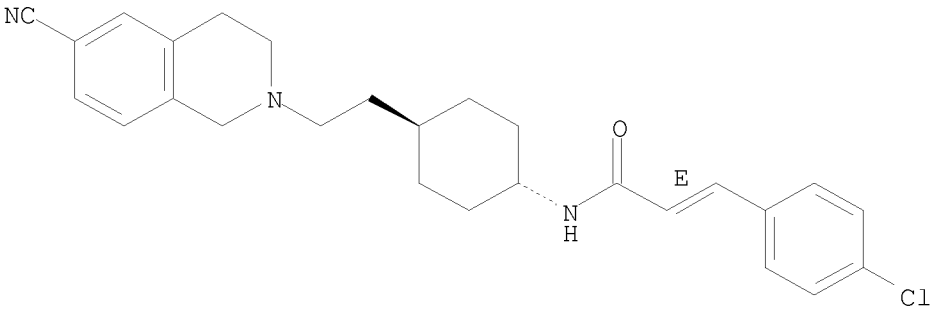
RN 215802-94-1 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-methoxyphenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



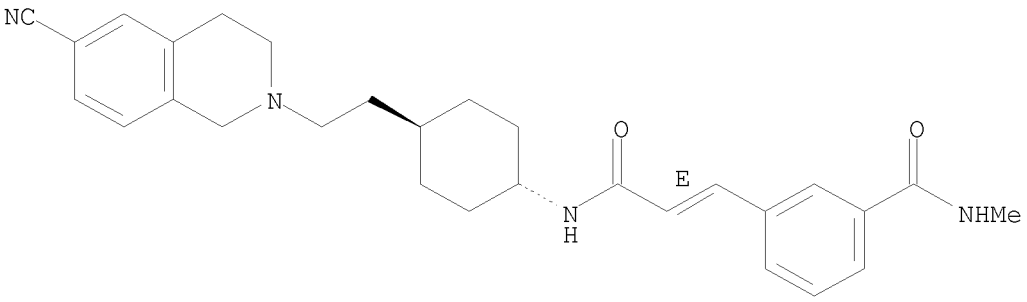
RN 215802-95-2 CAPLUS
CN 2-Propenamide, 3-(4-chlorophenyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



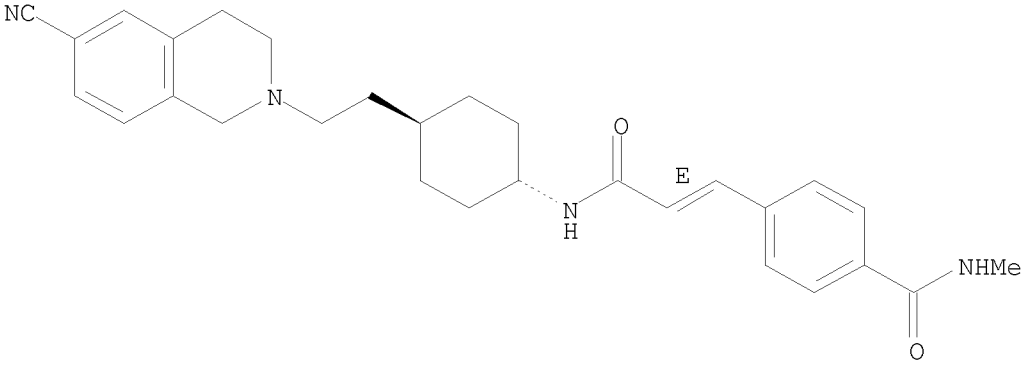
RN 215802-96-3 CAPLUS
CN Benzamide, 3-[(1E)-3-[[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]amino]-3-oxo-1-propen-1-yl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



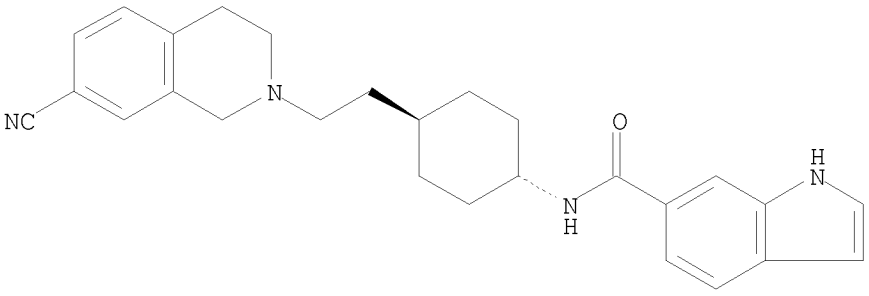
RN 215802-97-4 CAPLUS
CN Benzamide, 4-[(1E)-3-[[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]amino]-3-oxo-1-propen-1-yl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



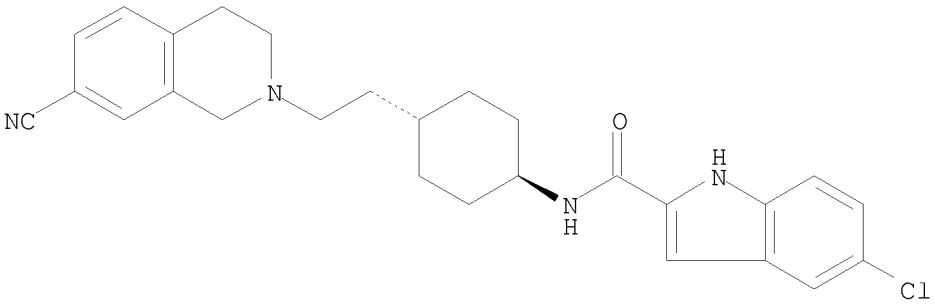
RN 215802-99-6 CAPLUS
CN 1H-Indole-6-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



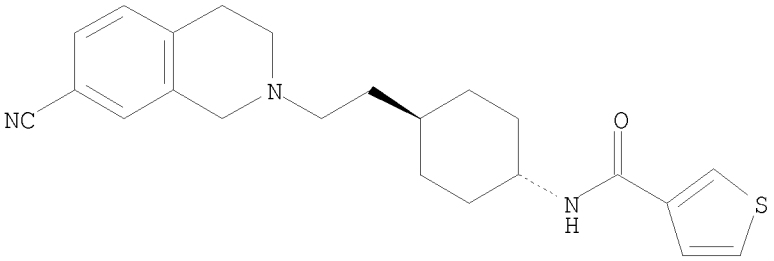
RN 215803-01-3 CAPLUS
CN 1H-Indole-2-carboxamide, 5-chloro-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



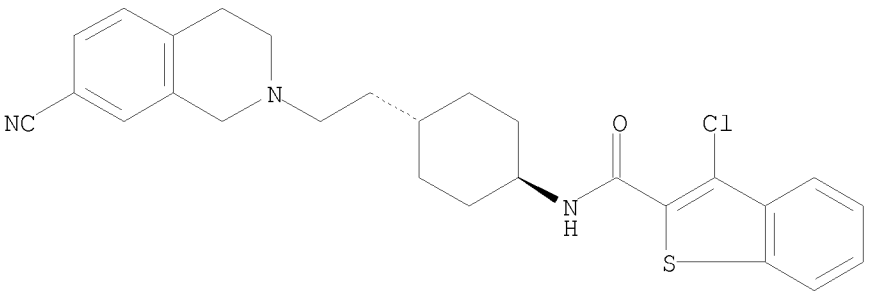
RN 215803-03-5 CAPLUS
CN 3-Thiophenecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



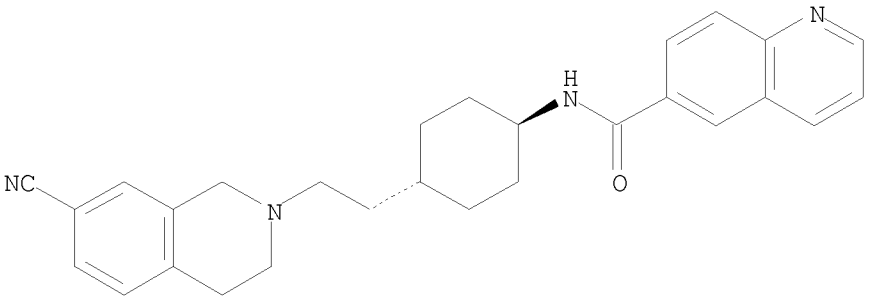
RN 215803-05-7 CAPLUS
CN Benzo[b]thiophene-2-carboxamide, 3-chloro-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



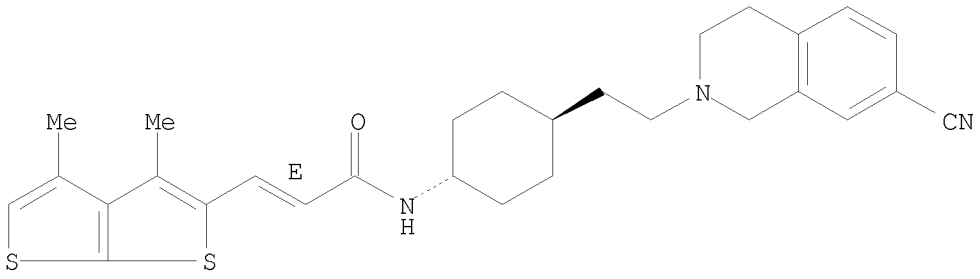
RN 215803-07-9 CAPLUS
CN 6-Quinolinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



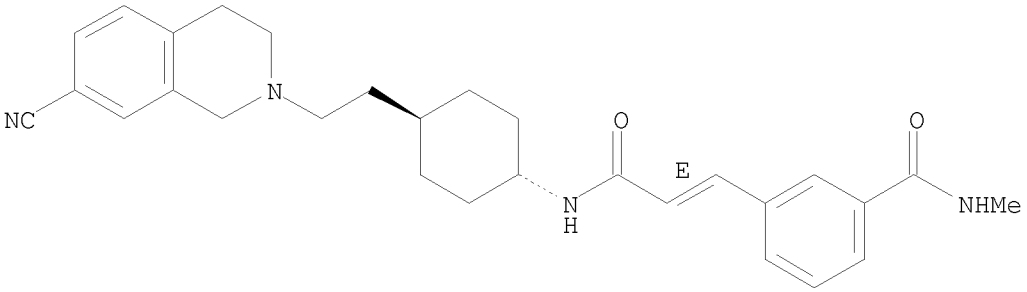
RN 215803-09-1 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3,4-dimethylthieno[2,3-b]thien-2-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



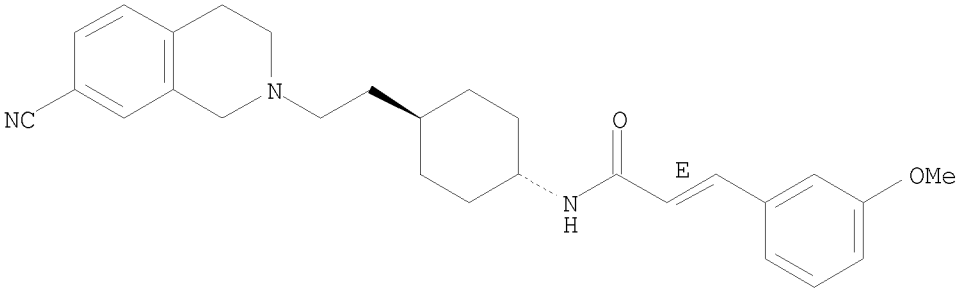
RN 215803-11-5 CAPLUS
CN Benzamide, 3-[(1E)-3-[[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]amino]-3-oxo-1-propen-1-yl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



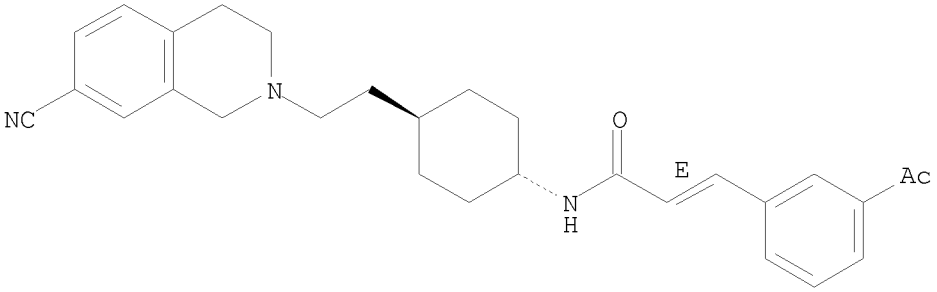
RN 215803-13-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3-methoxyphenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 215803-15-9 CAPLUS
CN 2-Propenamide, 3-(3-acetylphenyl)-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

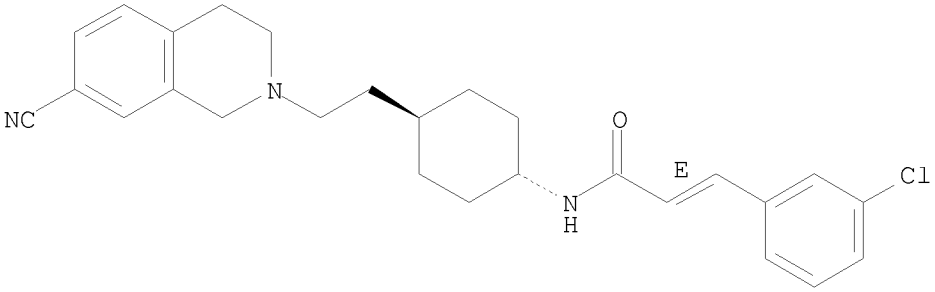
Relative stereochemistry.
Double bond geometry as shown.



RN 215803-17-1 CAPLUS
CN 2-Propenamide, 3-(3-chlorophenyl)-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-

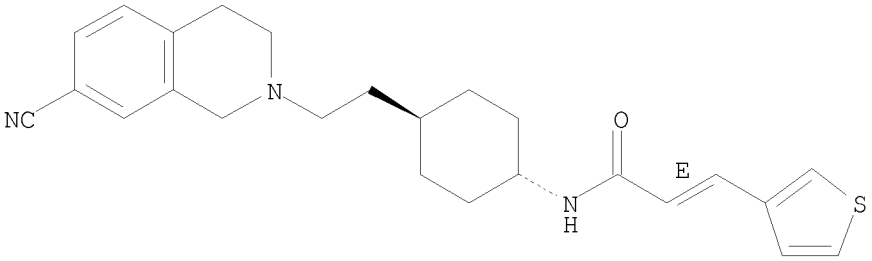
isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



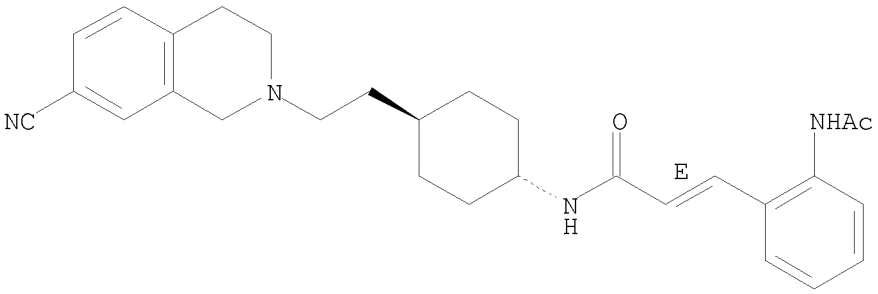
RN 215803-19-3 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3-thienyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



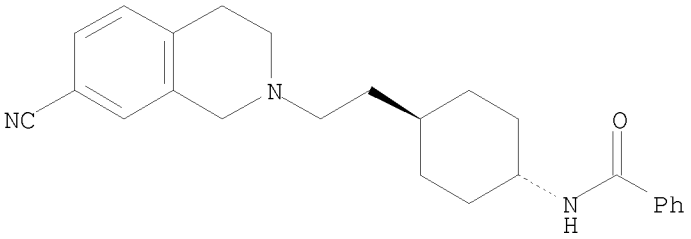
RN 215803-21-7 CAPLUS
CN 2-Propenamide, 3-[2-(acetylamino)phenyl]-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



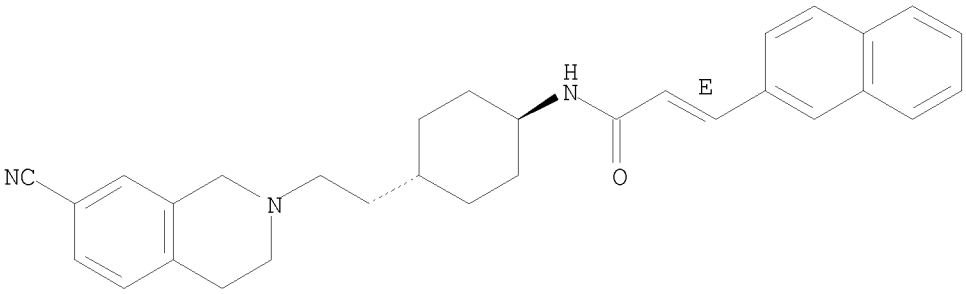
RN 215803-22-8 CAPLUS
CN Benzamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



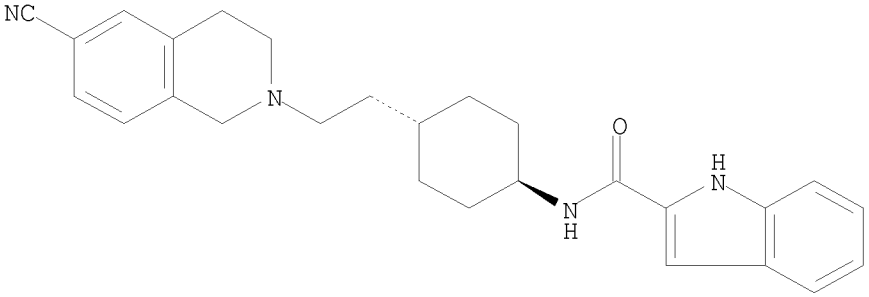
RN 215803-24-0 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-naphthalenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



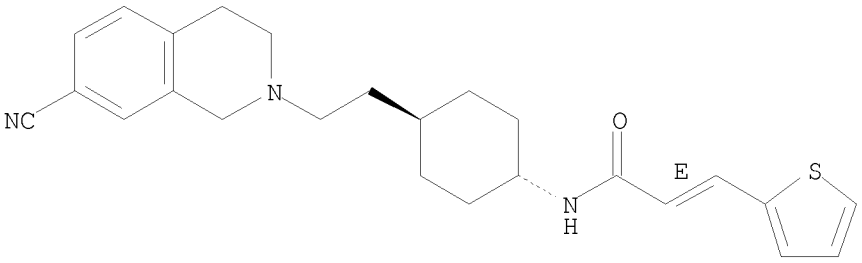
RN 215803-25-1 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



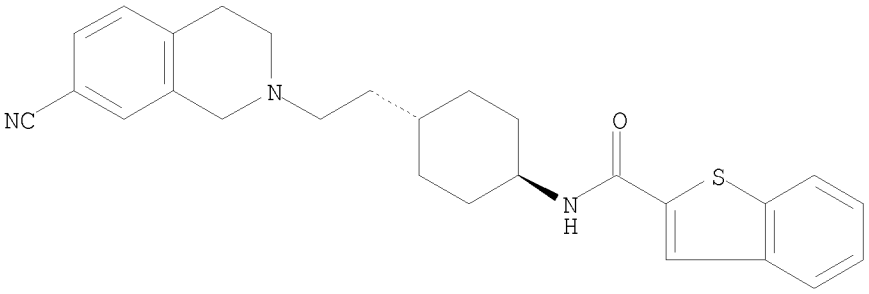
RN 215803-26-2 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-thienyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



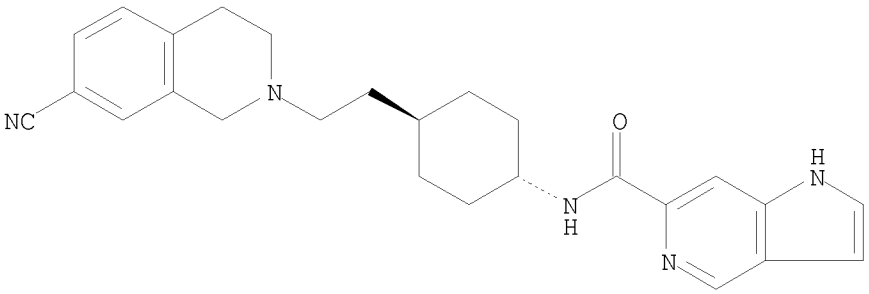
RN 215803-27-3 CAPLUS
CN Benzo[b]thiophene-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



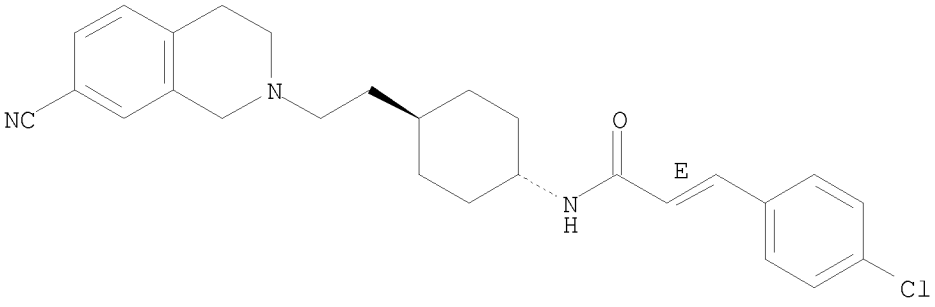
RN 215803-28-4 CAPLUS
CN 1H-Pyrrolo[3,2-c]pyridine-6-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



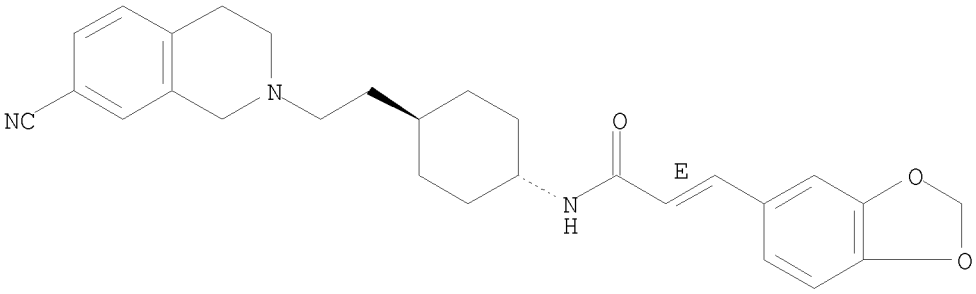
RN 215803-29-5 CAPLUS
CN 2-Propenamide, 3-(4-chlorophenyl)-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



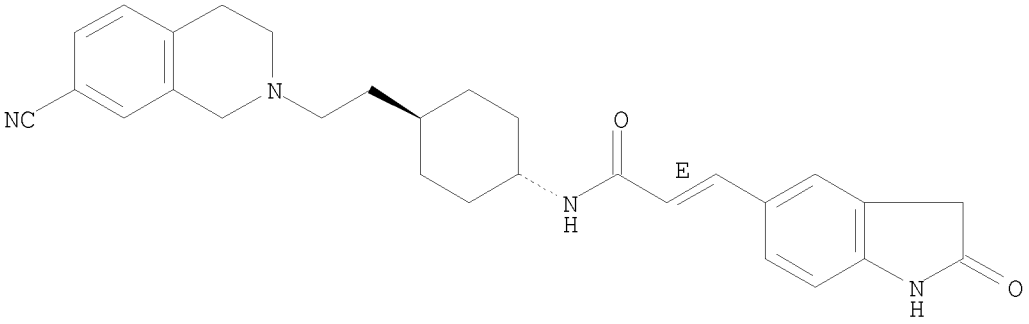
RN 215803-30-8 CAPLUS
CN 2-Propenamide, 3-(1,3-benzodioxol-5-yl)-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



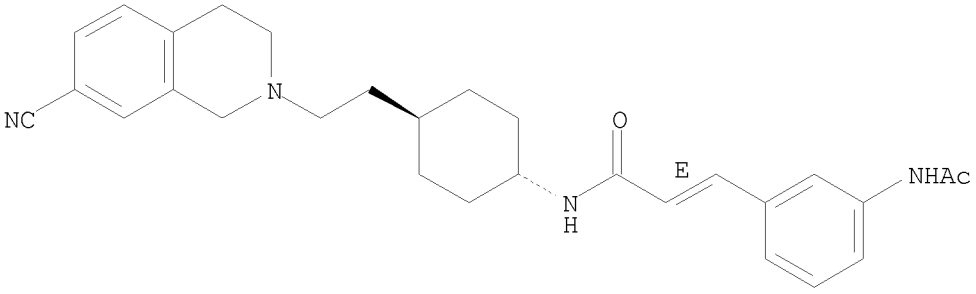
RN 215803-31-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2,3-dihydro-2-oxo-1H-indol-5-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



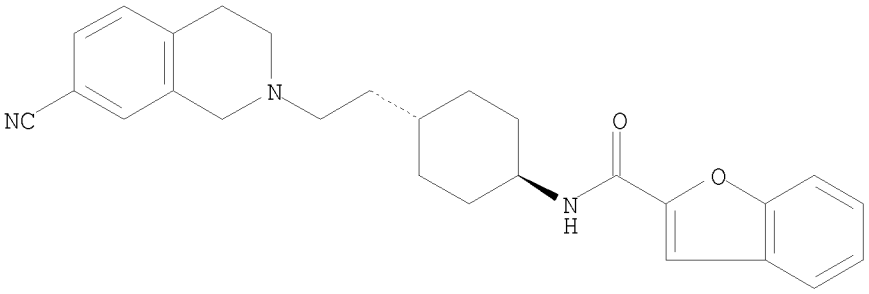
RN 215803-32-0 CAPLUS
CN 2-Propenamide, 3-[3-(acetylamino)phenyl]-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



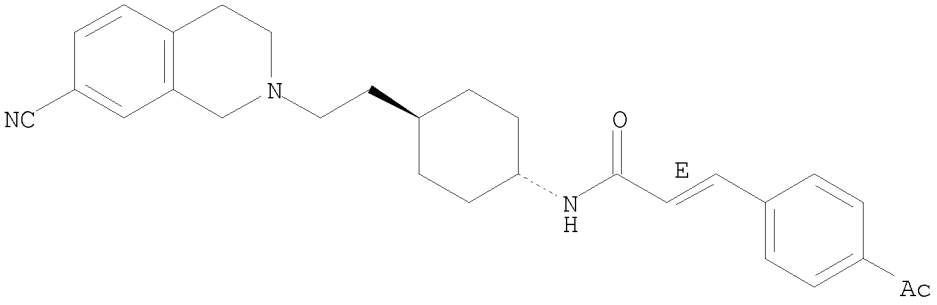
RN 215803-33-1 CAPLUS
CN 2-Benzofurancarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



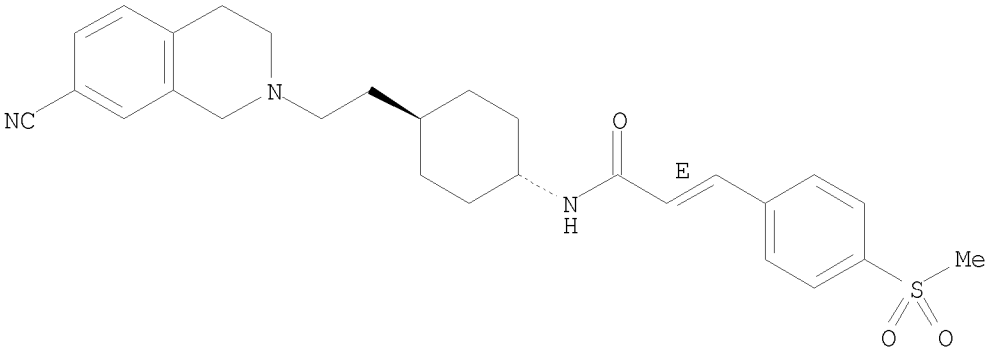
RN 215803-35-3 CAPLUS
CN 2-Propenamide, 3-(4-acetylphenyl)-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



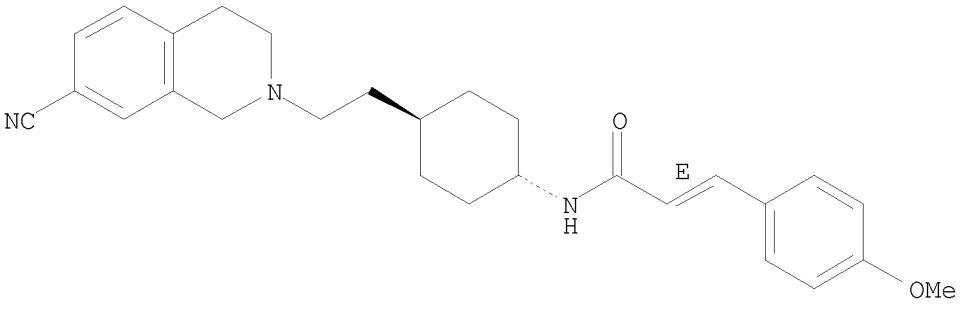
RN 215803-36-4 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[4-(methylsulfonyl)phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



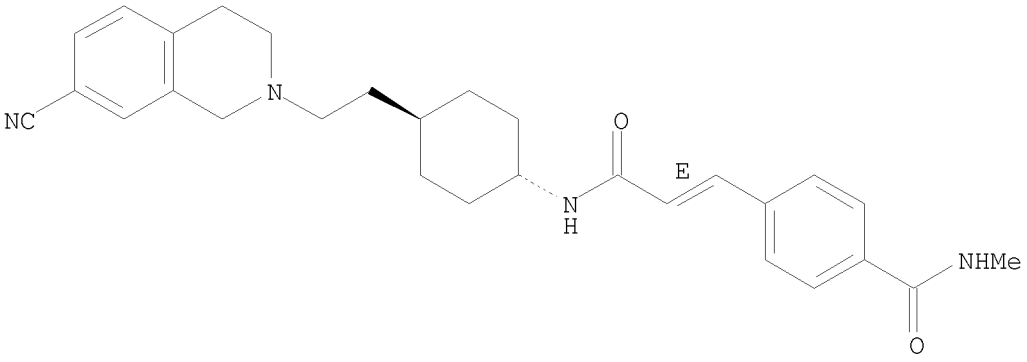
RN 215803-37-5 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-methoxyphenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



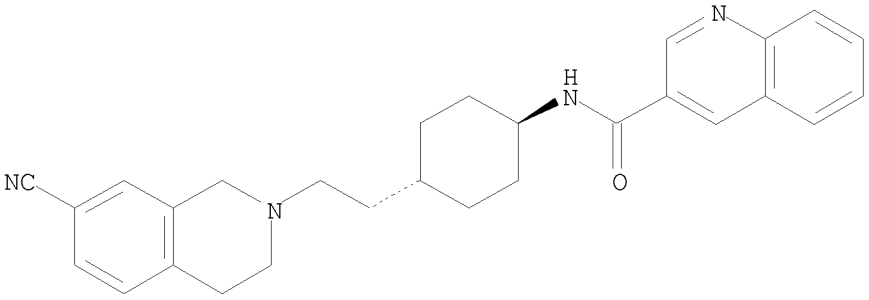
RN 215803-38-6 CAPLUS
CN Benzamide, 4-[(1E)-3-[[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]amino]-3-oxo-1-propen-1-yl]-N-methyl- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



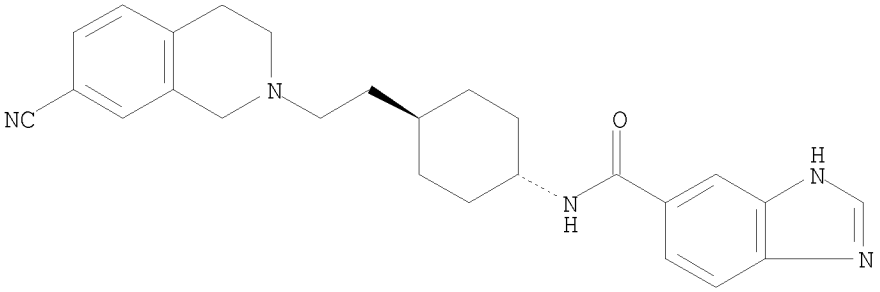
RN 215803-40-0 CAPLUS
CN 3-Quinolinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



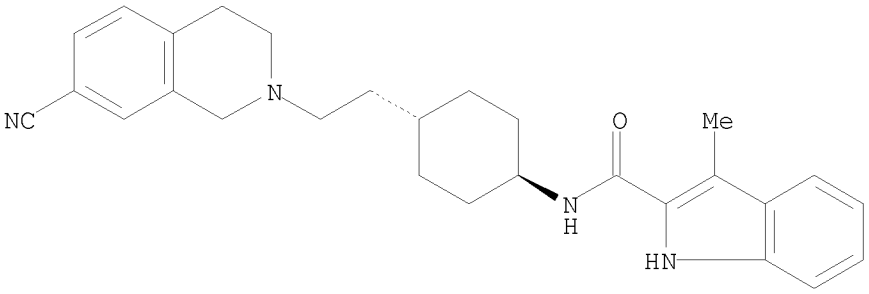
RN 215803-41-1 CAPLUS
CN 1H-Benzimidazole-6-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



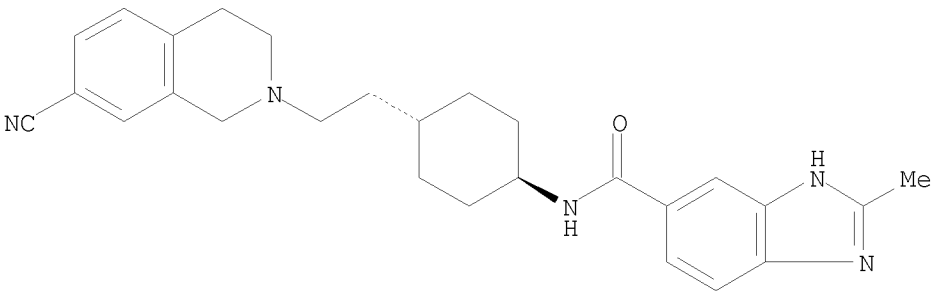
RN 215803-42-2 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-methyl- (CA INDEX NAME)

Relative stereochemistry.



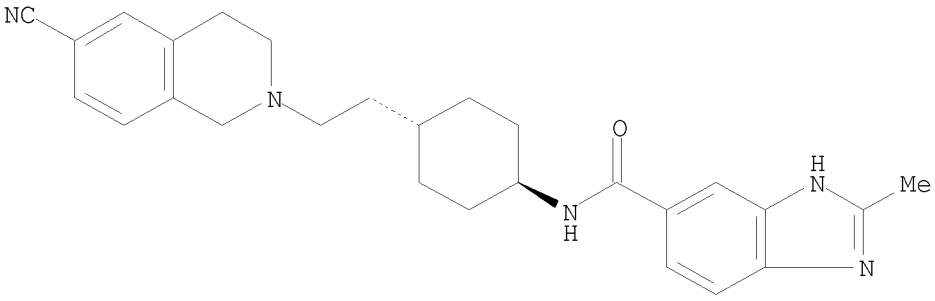
RN 215803-43-3 CAPLUS
CN 1H-Benzimidazole-6-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2-methyl- (CA INDEX NAME)

Relative stereochemistry.



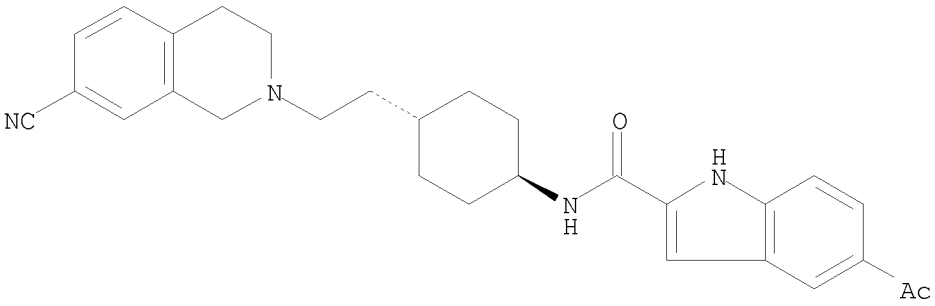
RN 215803-45-5 CAPLUS
CN 1H-Benzimidazole-6-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2-methyl- (CA INDEX NAME)

Relative stereochemistry.



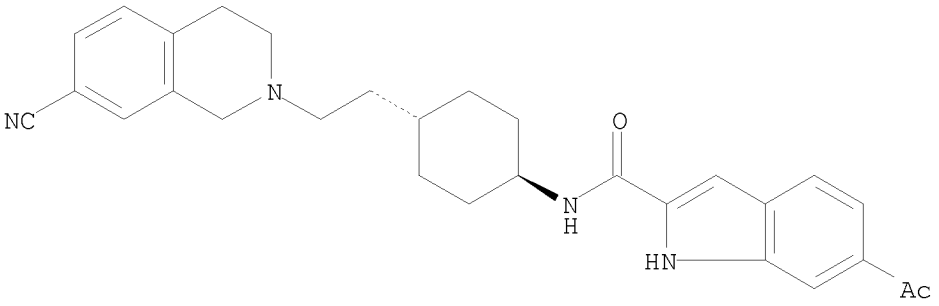
RN 215803-46-6 CAPLUS
CN 1H-Indole-2-carboxamide, 5-acetyl-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



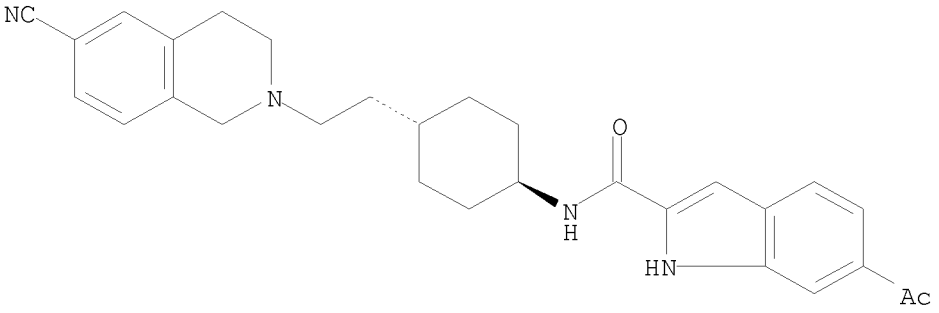
RN 215803-47-7 CAPLUS
CN 1H-Indole-2-carboxamide, 6-acetyl-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



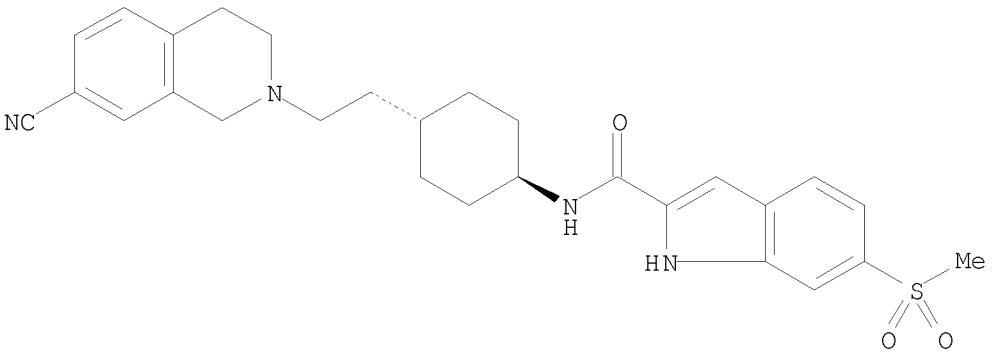
RN 215803-48-8 CAPLUS
CN 1H-Indole-2-carboxamide, 6-acetyl-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 215803-49-9 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-(methylsulfonyl)- (CA INDEX NAME)

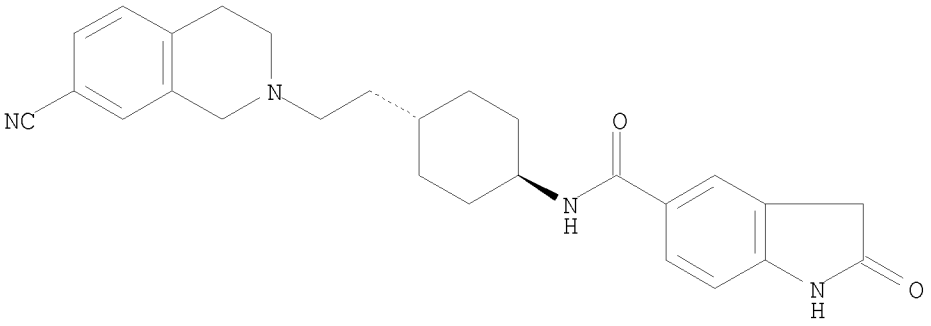
Relative stereochemistry.



RN 215803-50-2 CAPLUS

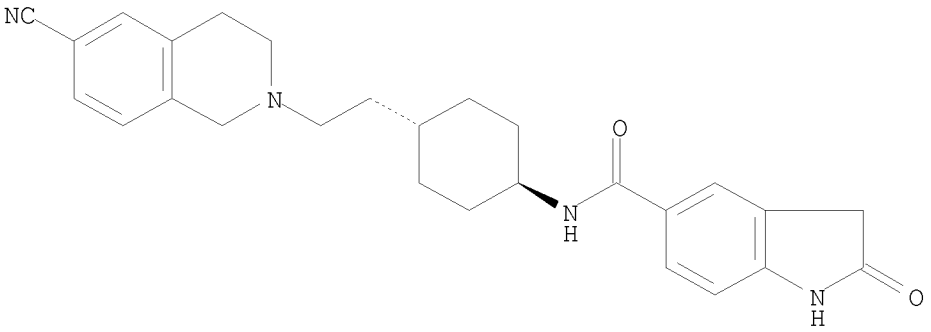
CN 1H-Indole-5-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2,3-dihydro-2-oxo- (CA INDEX NAME)

Relative stereochemistry.



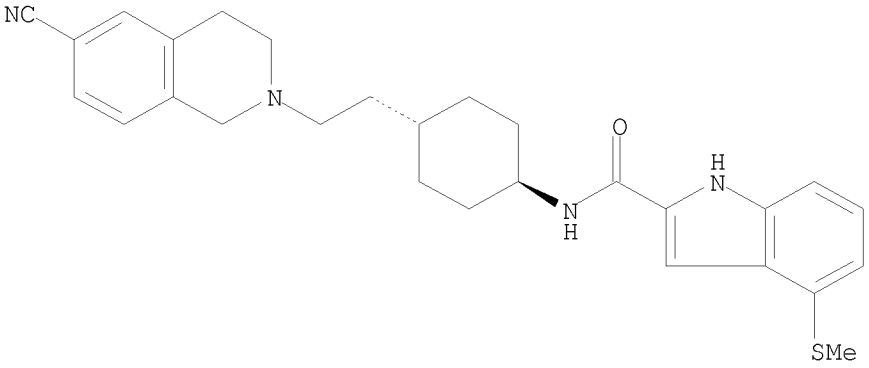
RN 215803-51-3 CAPLUS
CN 1H-Indole-5-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-2,3-dihydro-2-oxo- (CA INDEX NAME)

Relative stereochemistry.



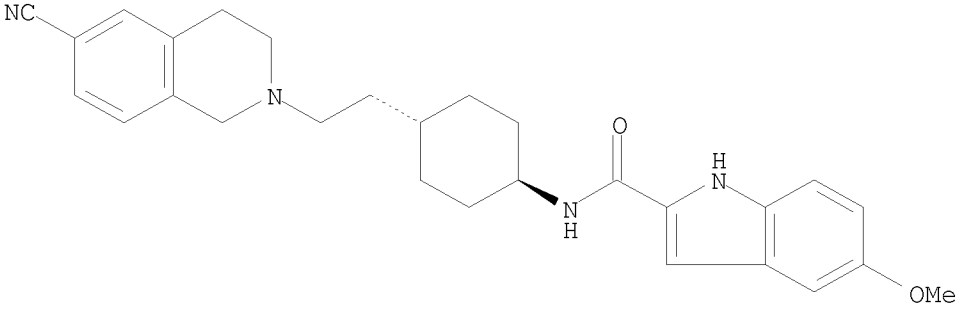
RN 215803-52-4 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-(methylthio)- (CA INDEX NAME)

Relative stereochemistry.



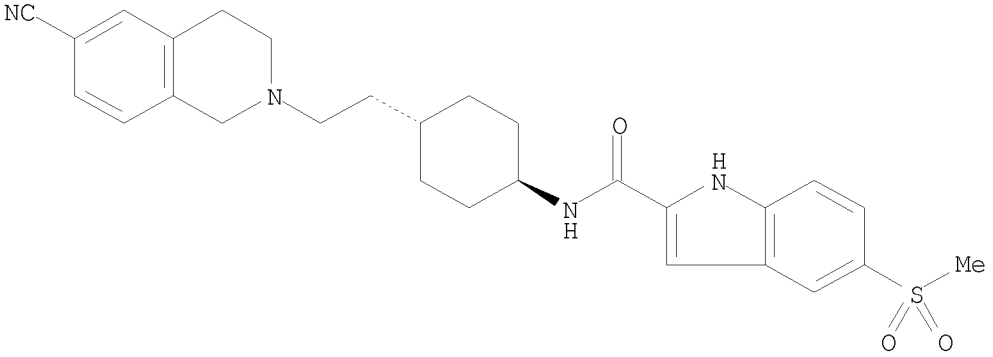
RN 215803-53-5 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-methoxy- (CA INDEX NAME)

Relative stereochemistry.



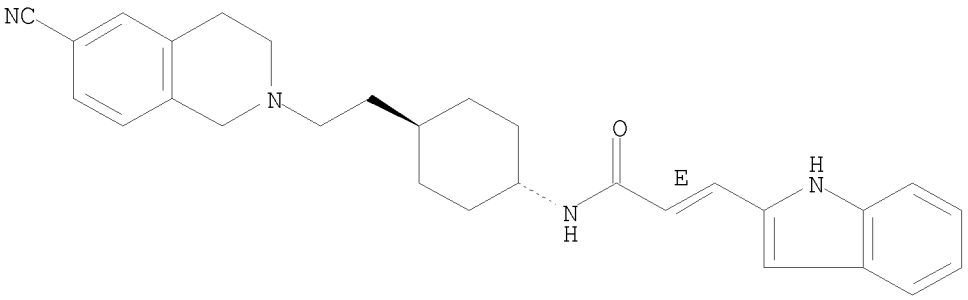
RN 215803-54-6 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-5-(methylsulfonyl)- (CA INDEX NAME)

Relative stereochemistry.



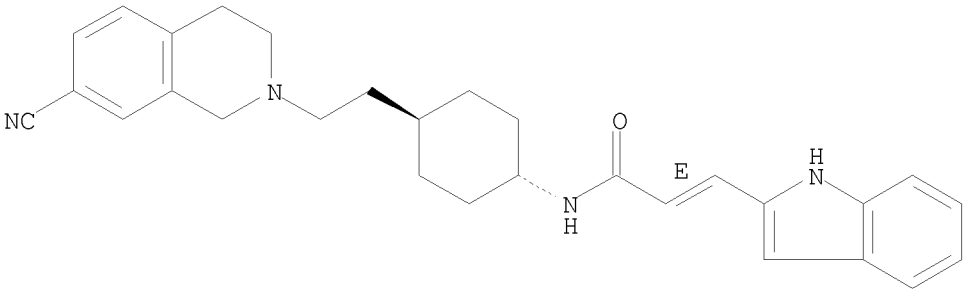
RN 215803-55-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(1H-indol-2-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



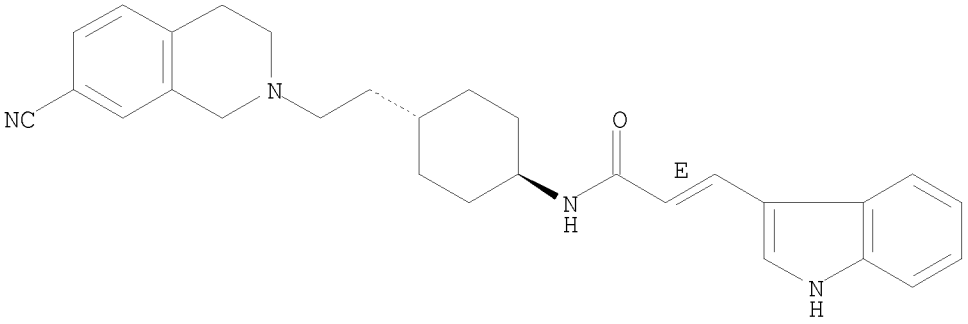
RN 215803-56-8 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(1H-indol-2-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



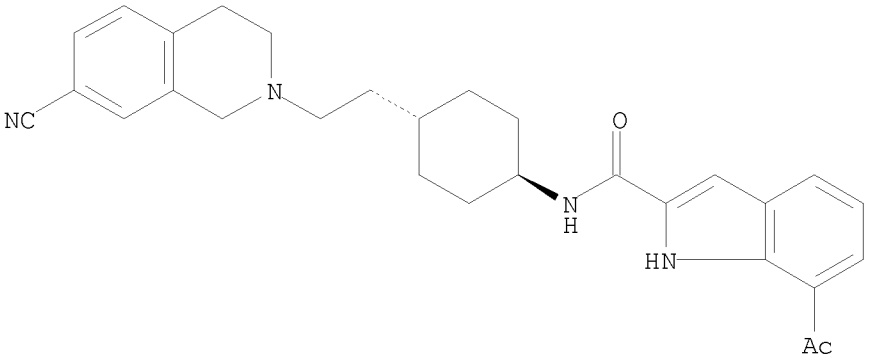
RN 215803-57-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(1H-indol-3-yl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



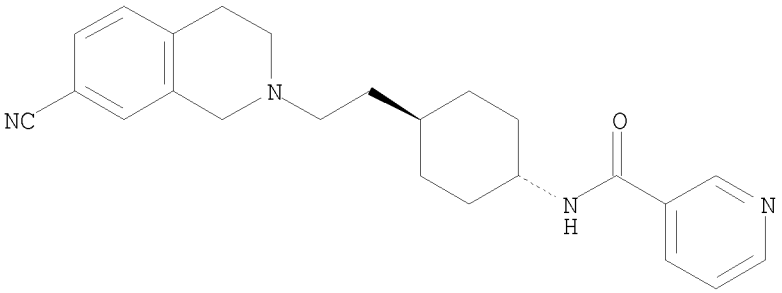
RN 215803-58-0 CAPLUS
CN 1H-Indole-2-carboxamide, 7-acetyl-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 215803-59-1 CAPLUS
CN 3-Pyridinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

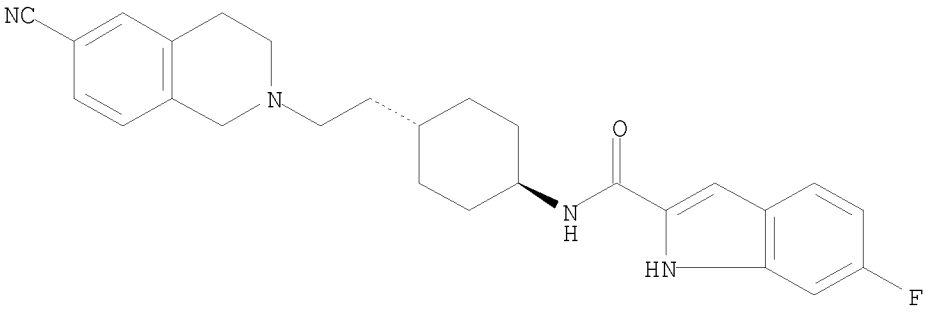
Relative stereochemistry.



RN 215803-60-4 CAPLUS

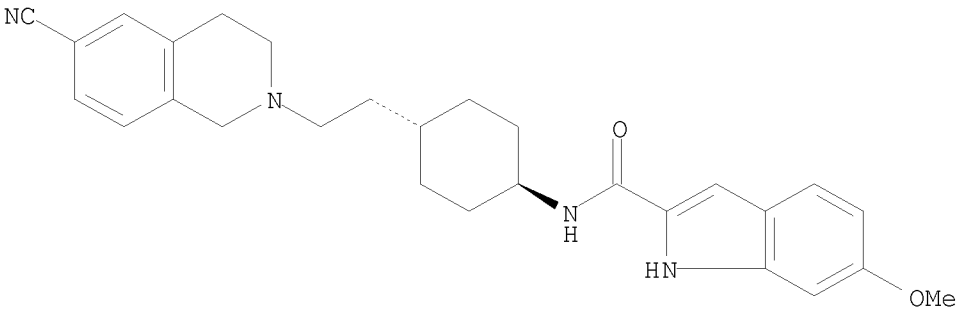
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-fluoro- (CA INDEX NAME)

Relative stereochemistry.



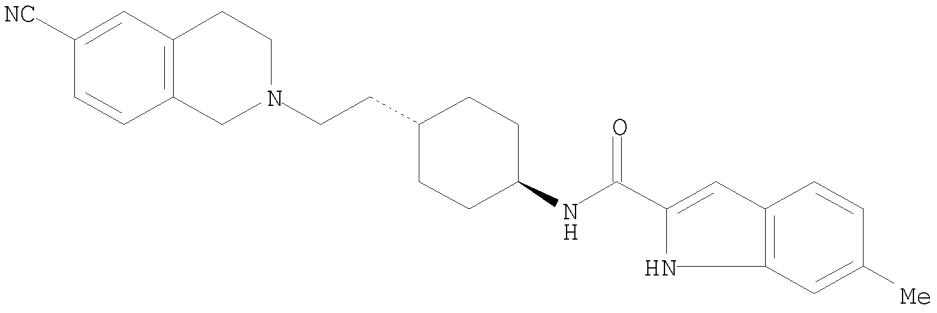
RN 215803-62-6 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-methoxy- (CA INDEX NAME)

Relative stereochemistry.



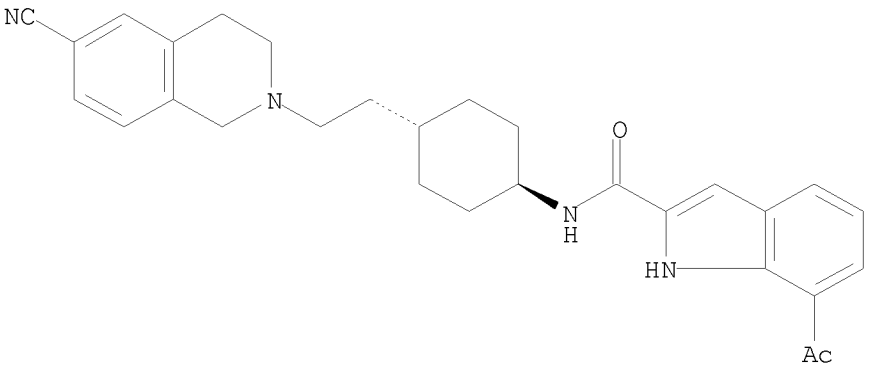
RN 215803-63-7 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-methyl- (CA INDEX NAME)

Relative stereochemistry.



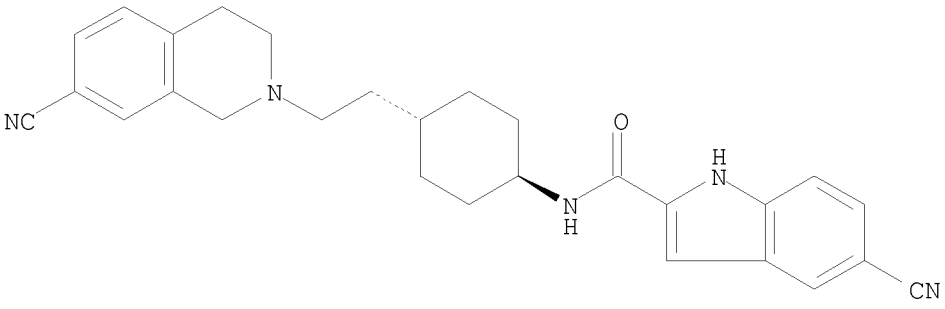
RN 215803-64-8 CAPLUS
CN 1H-Indole-2-carboxamide, 7-acetyl-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



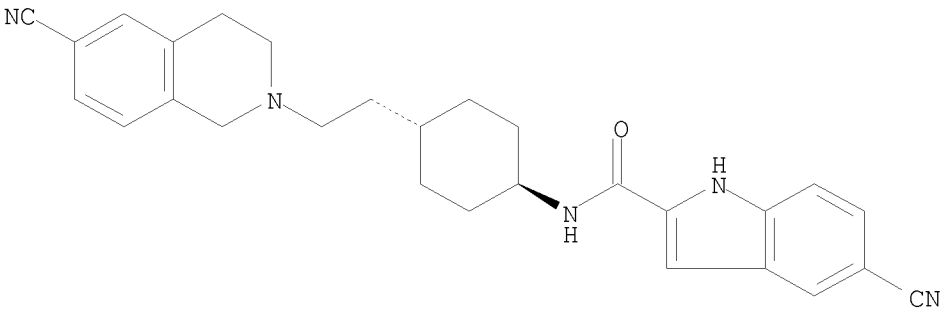
RN 215803-65-9 CAPLUS
CN 1H-Indole-2-carboxamide, 5-cyano-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



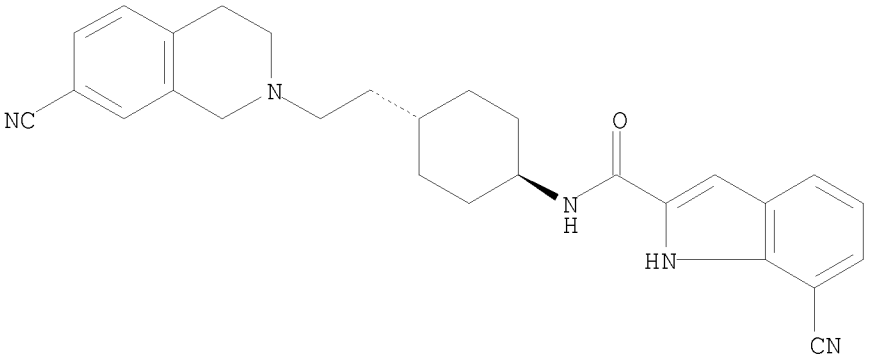
RN 215803-67-1 CAPLUS
CN 1H-Indole-2-carboxamide, 5-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



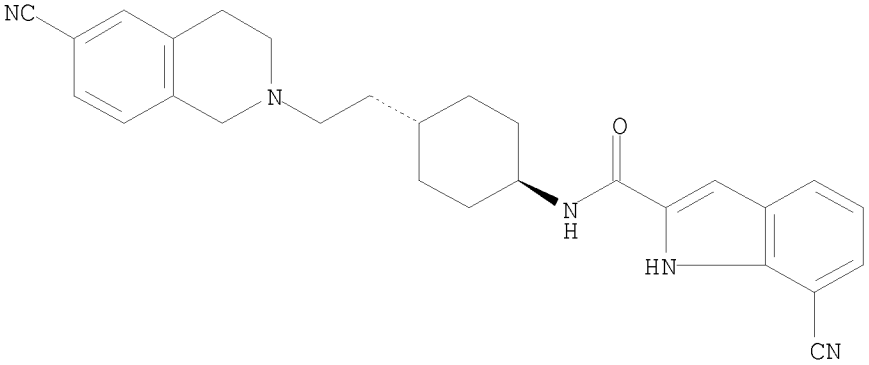
RN 215803-68-2 CAPLUS
CN 1H-Indole-2-carboxamide, 7-cyano-N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



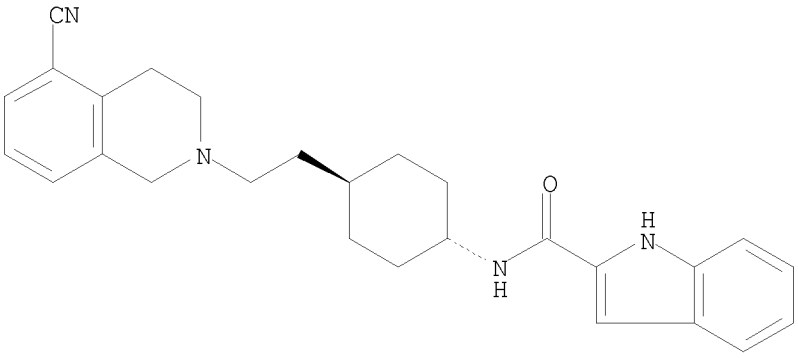
RN 215803-69-3 CAPLUS
CN 1H-Indole-2-carboxamide, 7-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



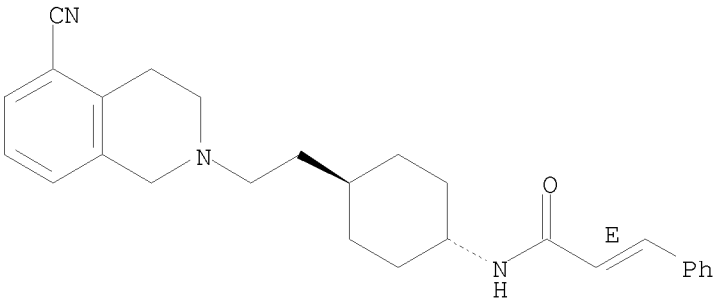
RN 215803-70-6 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(5-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



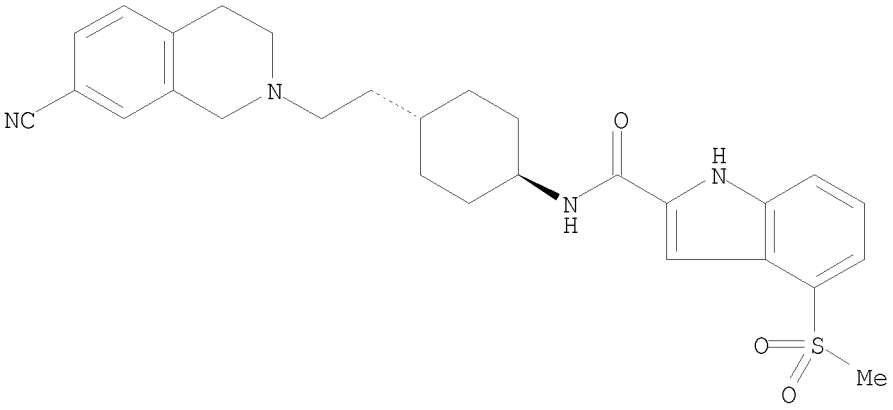
RN 215803-71-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(5-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



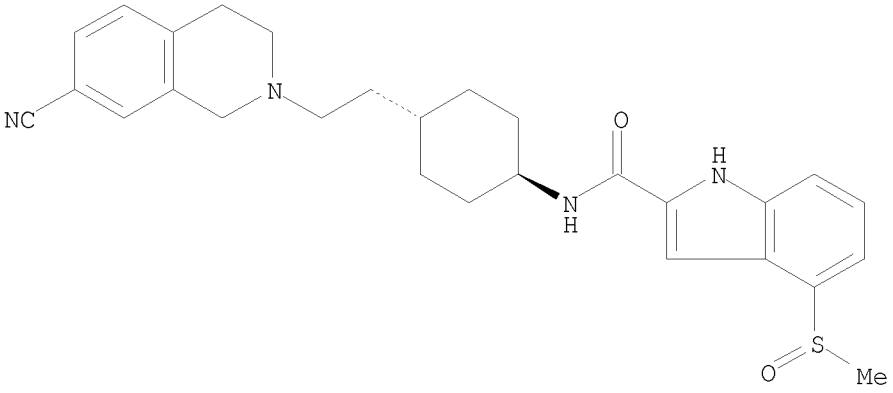
RN 215803-73-9 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-(methylsulfonyl)- (CA INDEX NAME)

Relative stereochemistry.



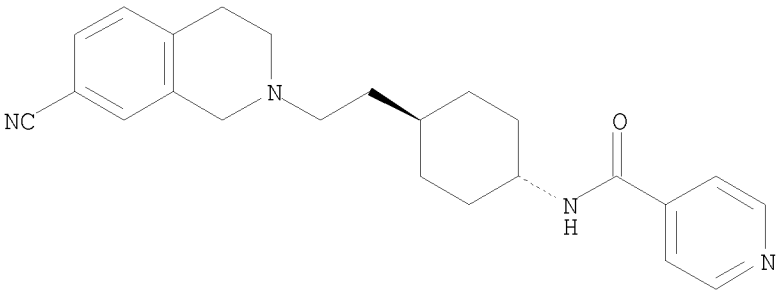
RN 215803-74-0 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-4-(methylsulfinyl)- (CA INDEX NAME)

Relative stereochemistry.



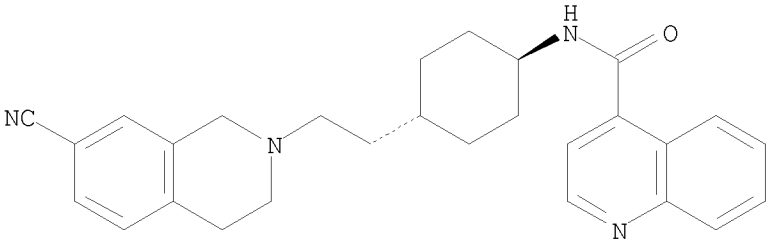
RN 215803-75-1 CAPLUS
CN 4-Pyridinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



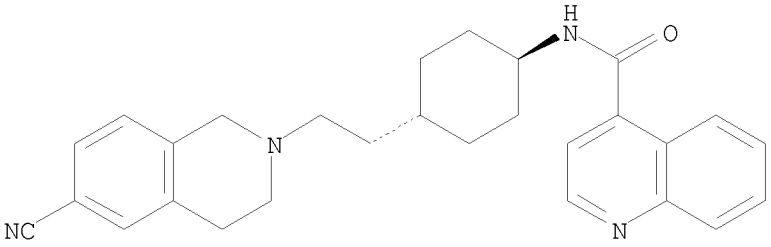
RN 215803-77-3 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



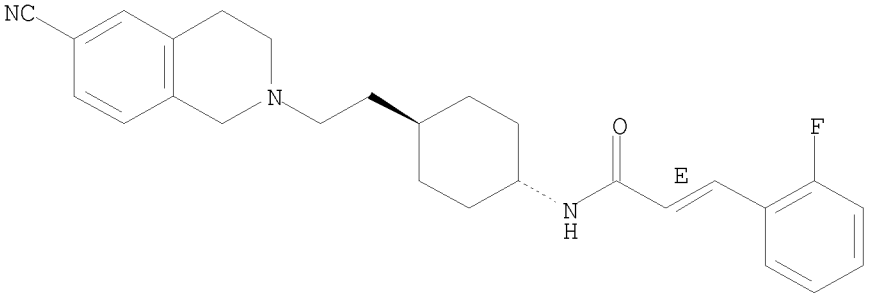
RN 215803-78-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



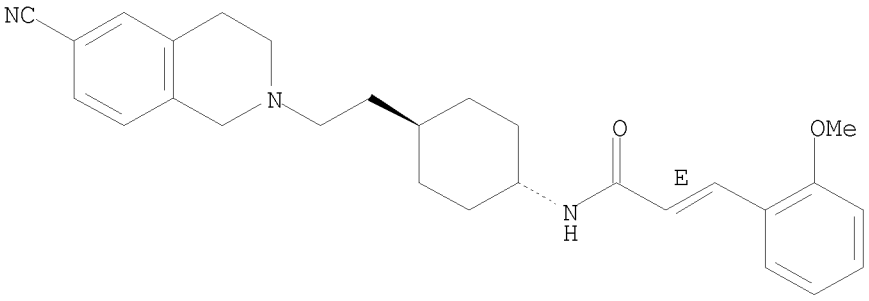
RN 215803-80-8 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-fluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



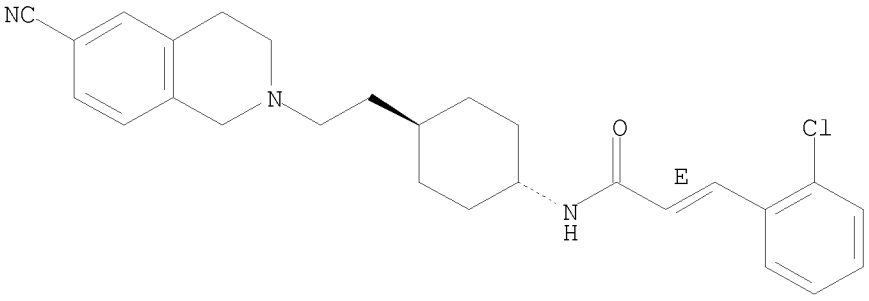
RN 215803-81-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-methoxyphenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



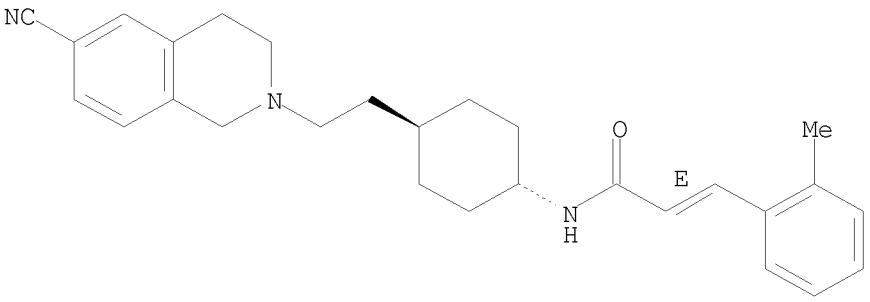
RN 215803-84-2 CAPLUS
CN 2-Propenamide, 3-(2-chlorophenyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



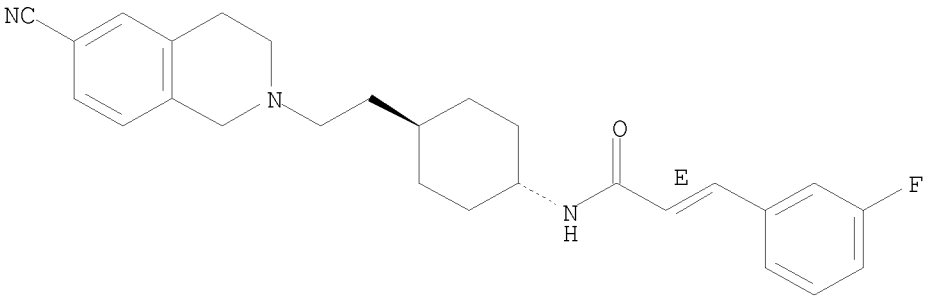
RN 215803-86-4 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2-methylphenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



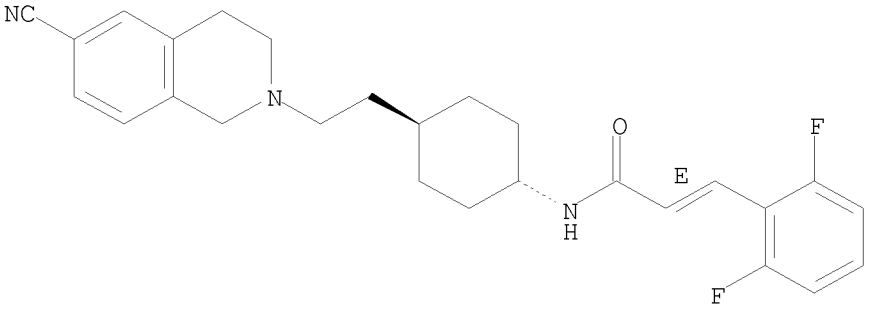
RN 215803-88-6 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3-fluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



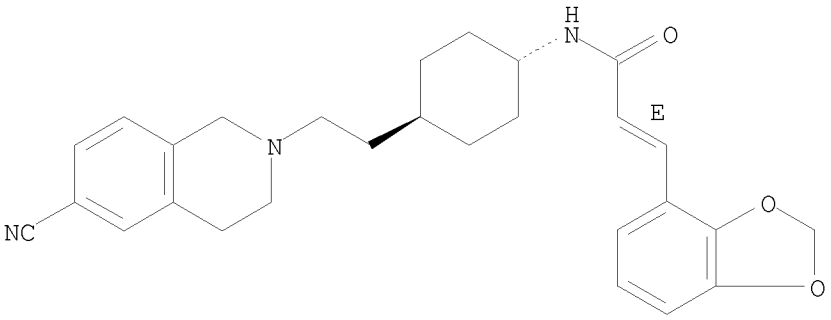
RN 215803-90-0 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2,6-difluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



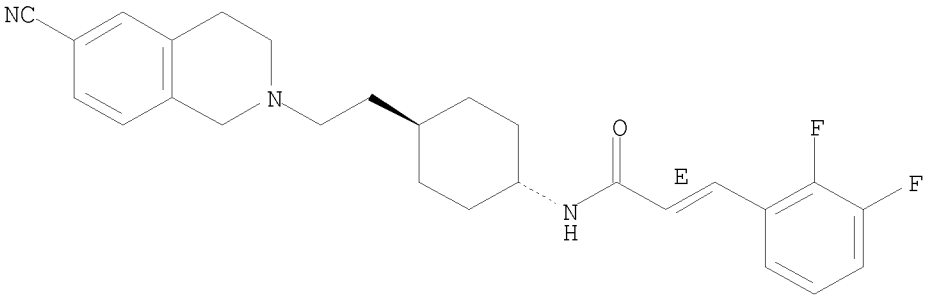
RN 215803-92-2 CAPLUS
CN 2-Propenamide, 3-(1,3-benzodioxol-4-yl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



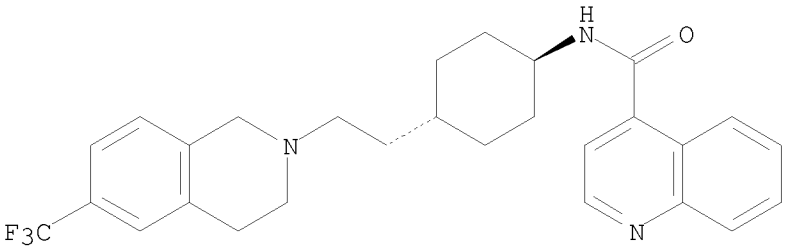
RN 215803-94-4 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2,3-difluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



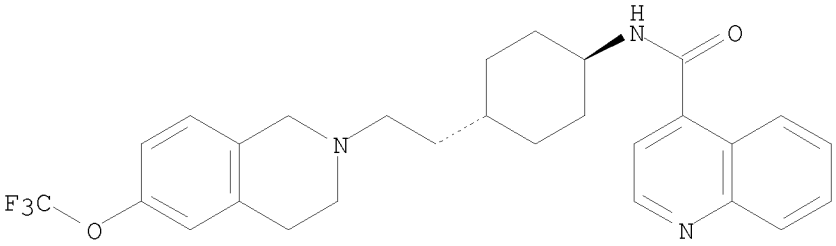
RN 215803-96-6 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-[3,4-dihydro-6-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



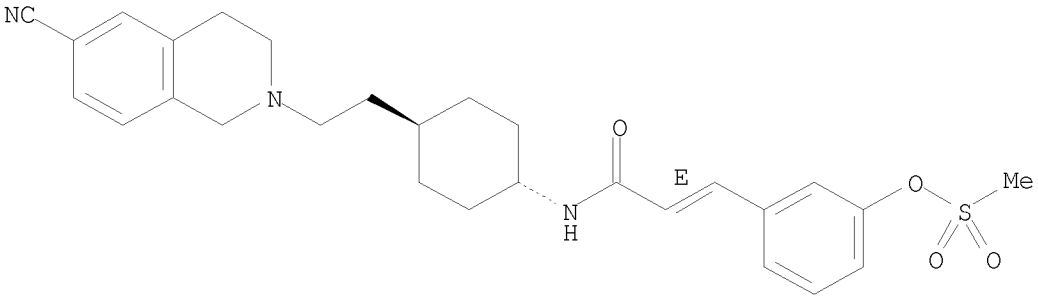
RN 215803-98-8 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-[3,4-dihydro-6-(trifluoromethoxy)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



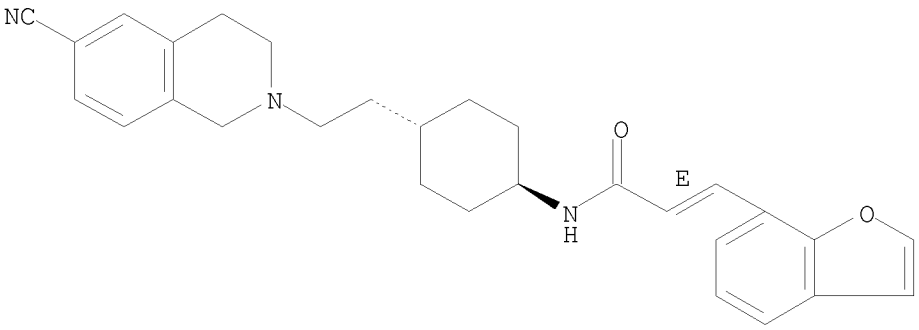
RN 215804-00-5 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[3-[(methylsulfonyl)oxy]phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



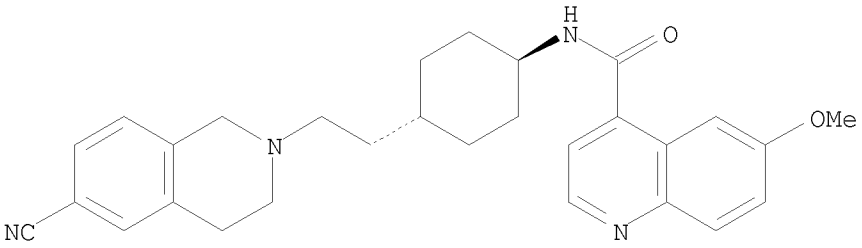
RN 215804-01-6 CAPLUS
CN 2-Propenamide, 3-(7-benzofuranyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



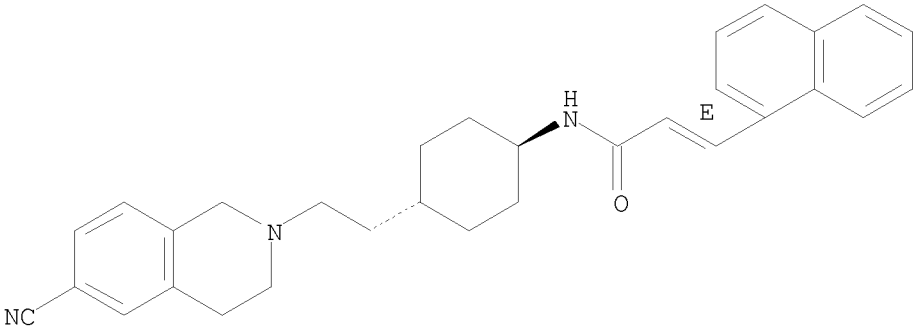
RN 215804-03-8 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-methoxy- (CA INDEX NAME)

Relative stereochemistry.



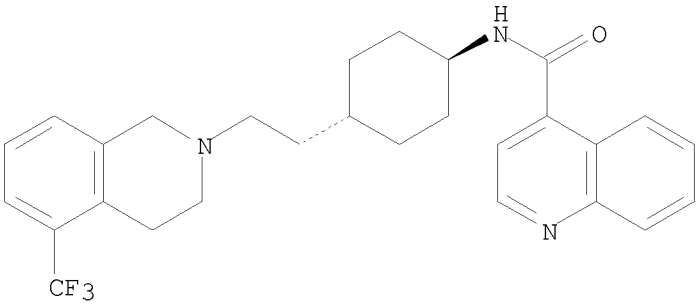
RN 215804-04-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(1-naphthalenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



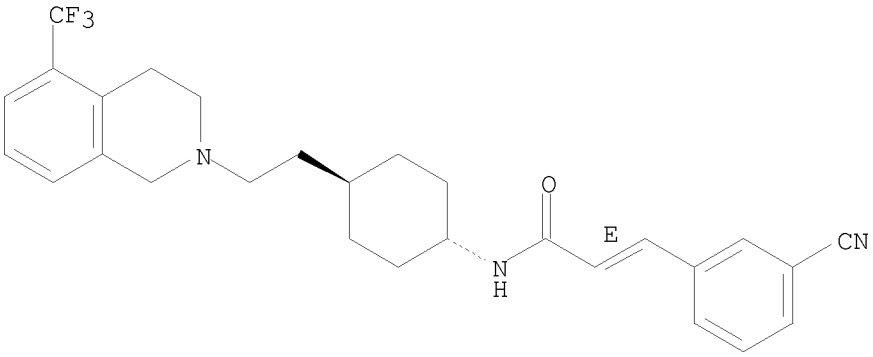
RN 215804-05-0 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



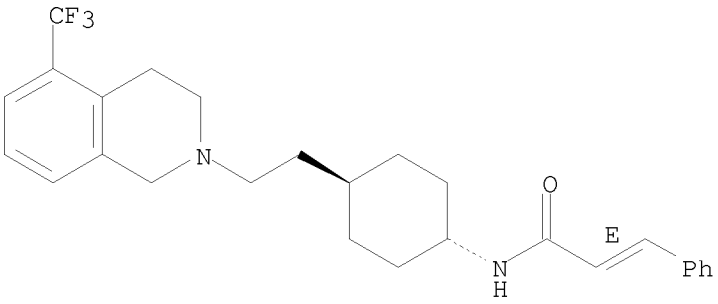
RN 215804-07-2 CAPLUS
CN 2-Propenamide, 3-(3-cyanophenyl)-N-[trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



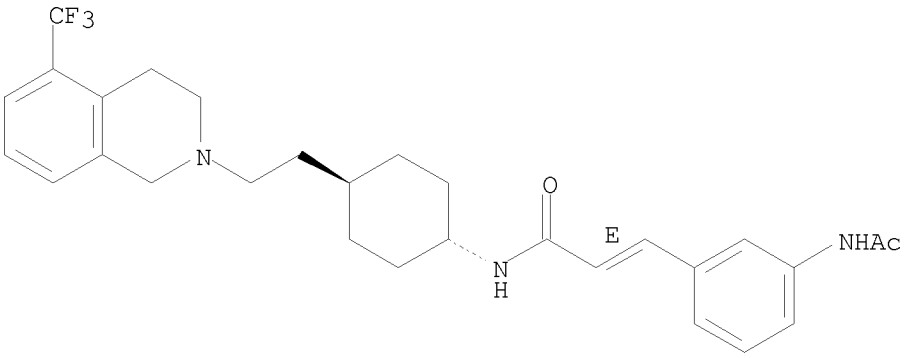
RN 215804-08-3 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



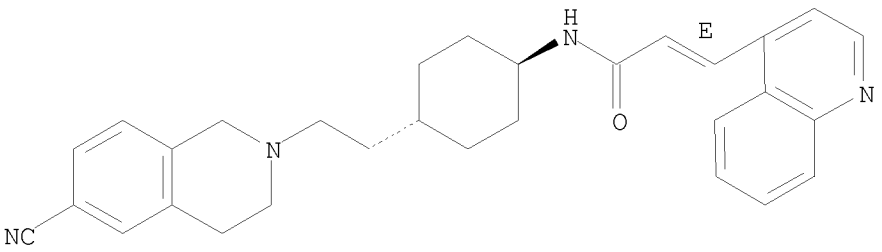
RN 215804-09-4 CAPLUS
CN 2-Propenamide, 3-[3-(acetylamino)phenyl]-N-[trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



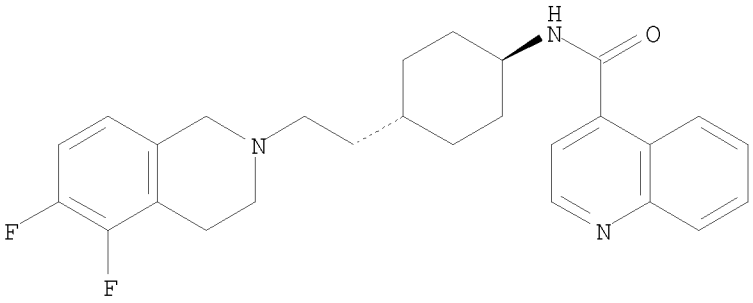
RN 215804-10-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-quinolinyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



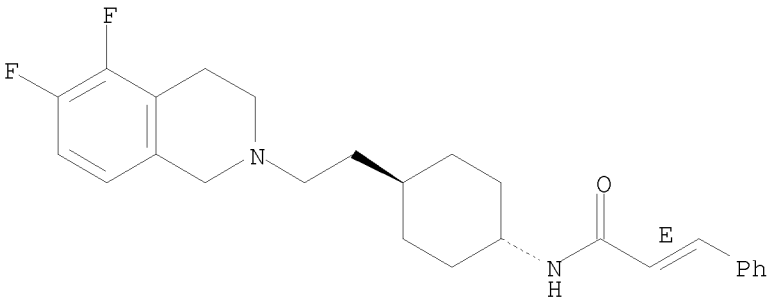
RN 215804-11-8 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(5,6-difluoro-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



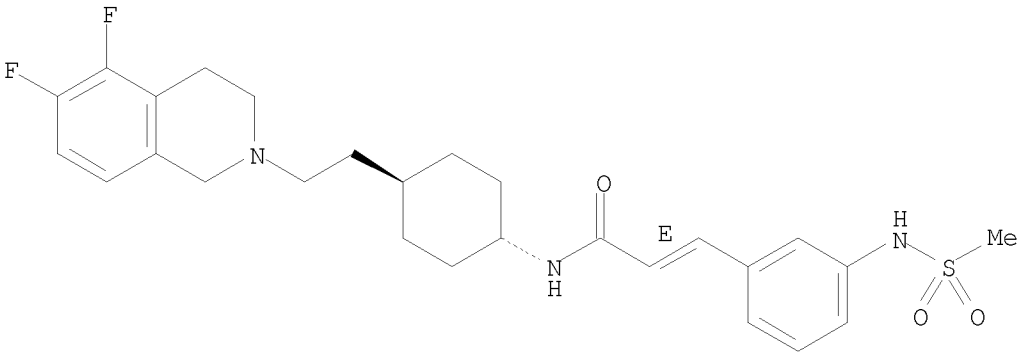
RN 215804-13-0 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(5,6-difluoro-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



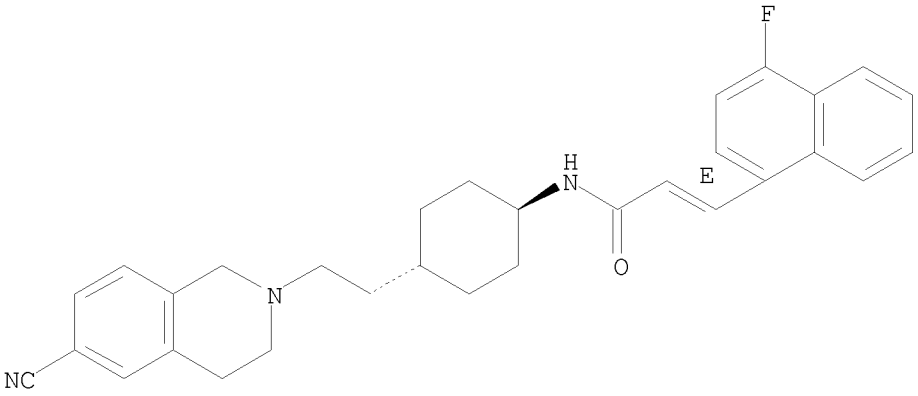
RN 215804-14-1 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(5,6-difluoro-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[3-[(methylsulfonyl)amino]phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



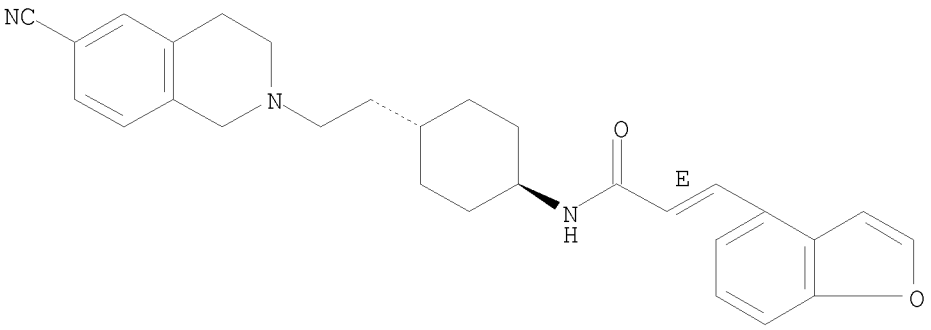
RN 215804-15-2 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-fluoro-1-naphthalenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



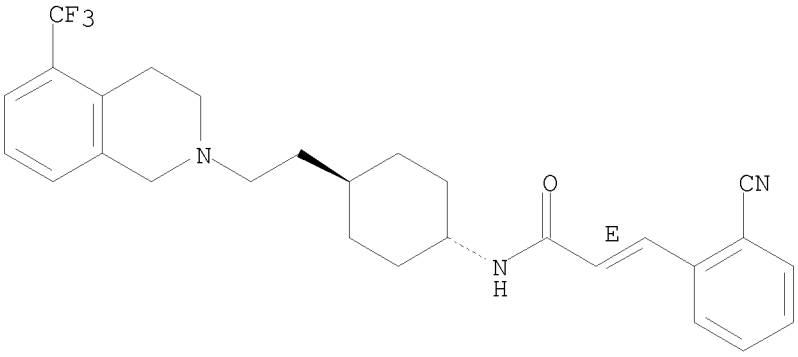
RN 215804-16-3 CAPLUS
CN 2-Propenamide, 3-(4-benzofuranyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



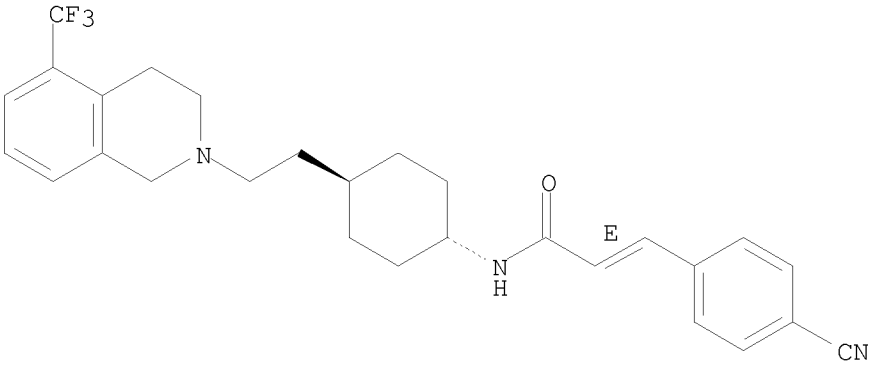
RN 215804-17-4 CAPLUS
CN 2-Propenamide, 3-(2-cyanophenyl)-N-[trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



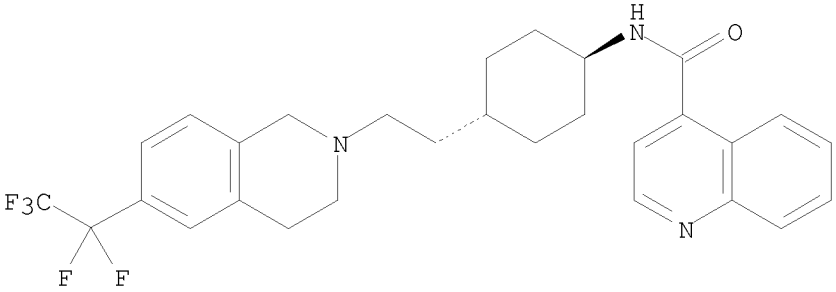
RN 215804-18-5 CAPLUS
CN 2-Propenamide, 3-(4-cyanophenyl)-N-[trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



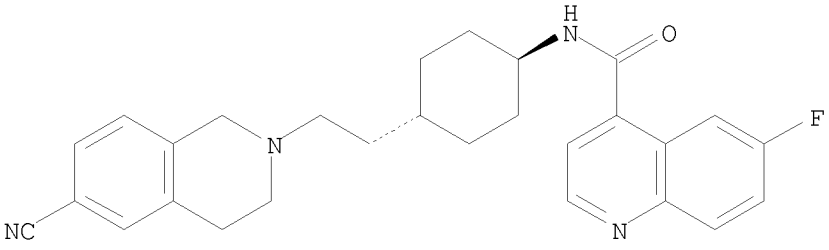
RN 215804-20-9 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-[3,4-dihydro-6-(1,1,2,2,2-pentafluoroethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



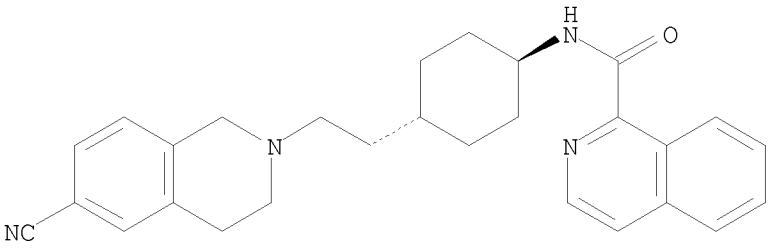
RN 215804-21-0 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-6-fluoro- (CA INDEX NAME)

Relative stereochemistry.



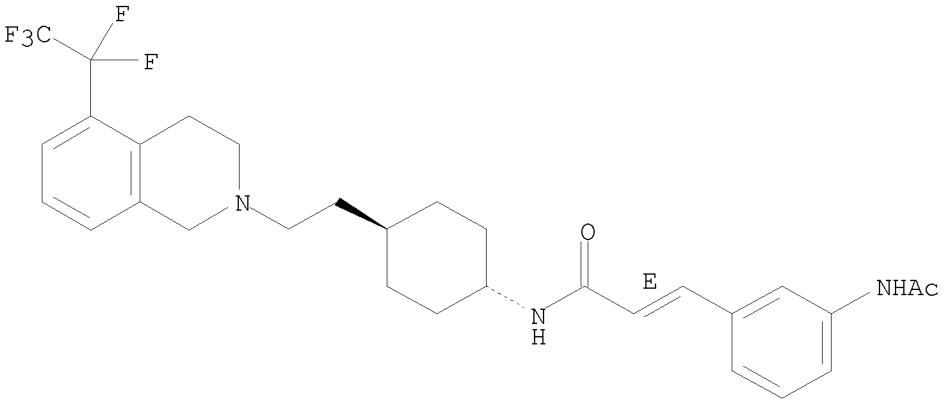
RN 215804-22-1 CAPLUS
CN 1-Isoquinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



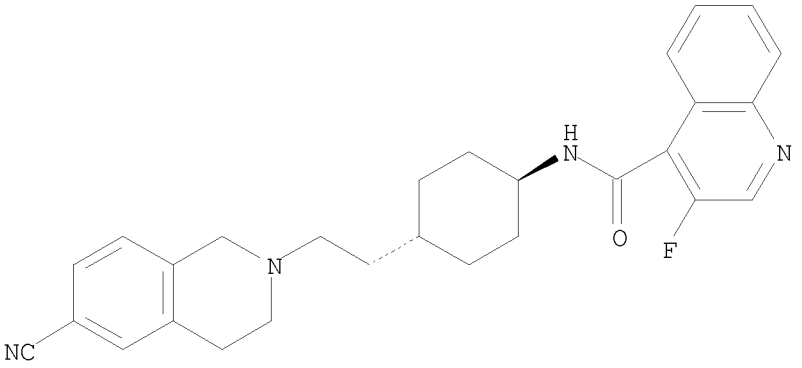
RN 215804-23-2 CAPLUS
CN 2-Propenamide, 3-[3-(acetylamino)phenyl]-N-[trans-4-[2-[3,4-dihydro-5-(1,1,2,2,2-pentafluoroethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



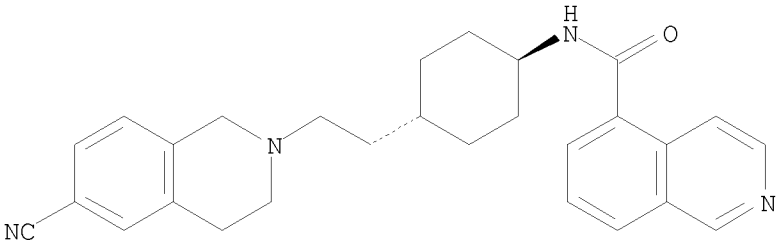
RN 215804-24-3 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-fluoro- (CA INDEX NAME)

Relative stereochemistry.



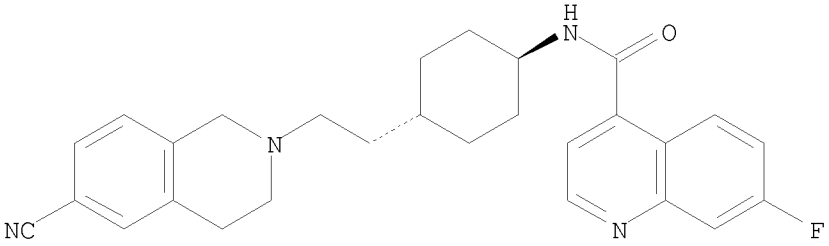
RN 215804-25-4 CAPLUS
CN 5-Isoquinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



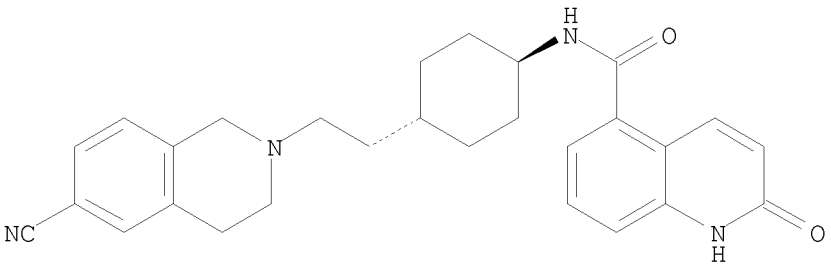
RN 215804-26-5 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-7-fluoro- (CA INDEX NAME)

Relative stereochemistry.



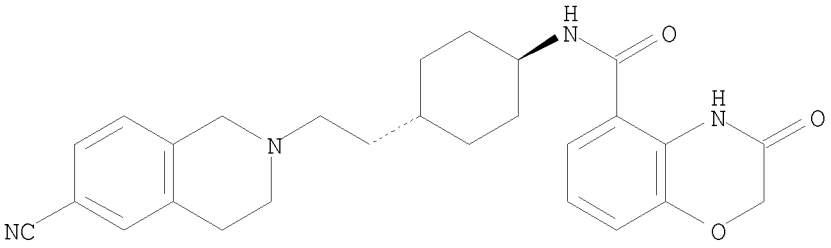
RN 215804-27-6 CAPLUS
CN 5-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-1,2-dihydro-2-oxo- (CA INDEX NAME)

Relative stereochemistry.



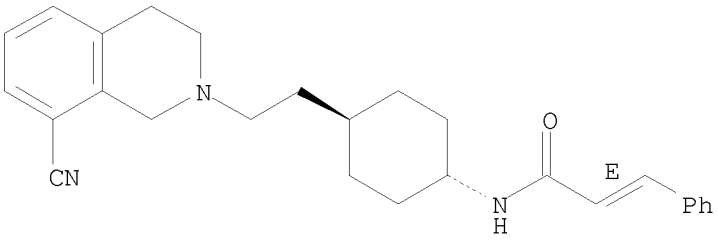
RN 215804-29-8 CAPLUS
CN 2H-1,4-Benzoxazine-5-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3,4-dihydro-3-oxo- (CA INDEX NAME)

Relative stereochemistry.



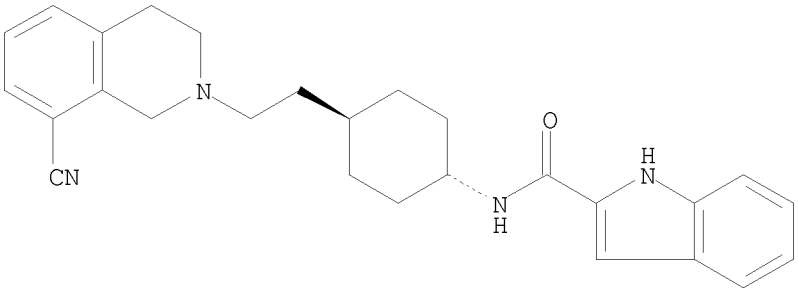
RN 215804-30-1 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(8-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



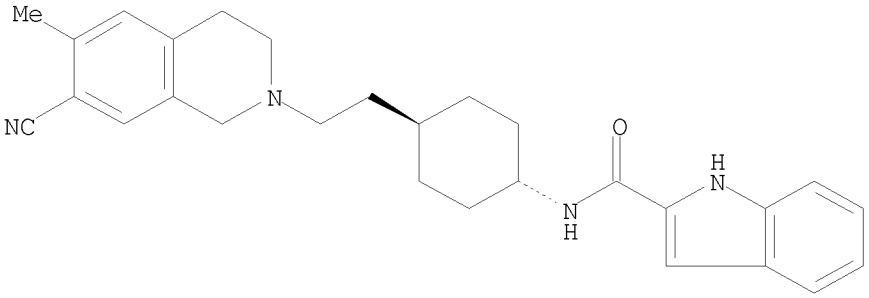
RN 215804-31-2 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(8-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



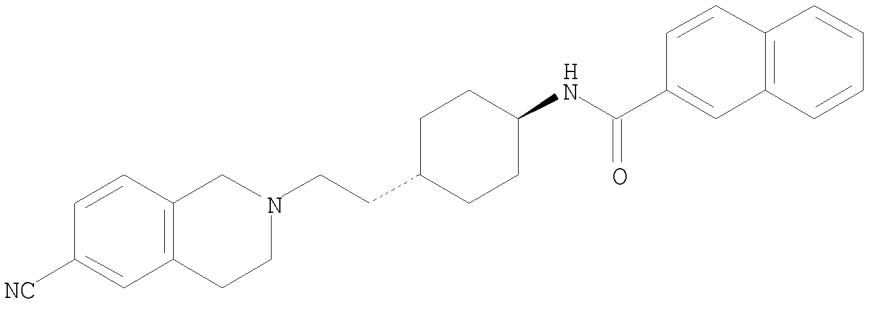
RN 215804-32-3 CAPLUS
CN 1H-Indole-2-carboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-6-methyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



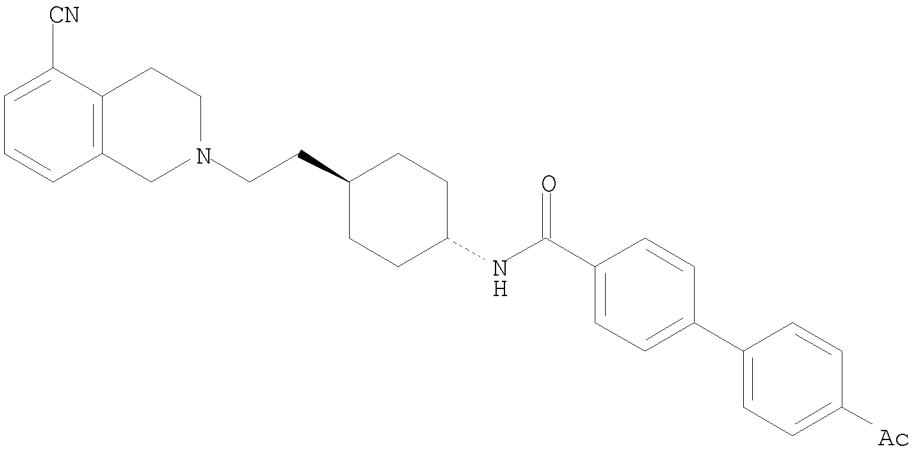
RN 215804-33-4 CAPLUS
CN 2-Naphthalenecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



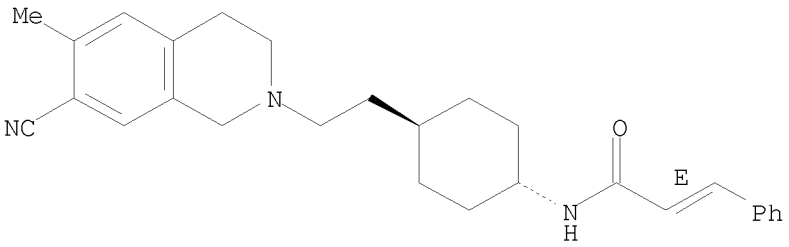
RN 215804-34-5 CAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, 4'-acetyl-N-[trans-4-[2-(5-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



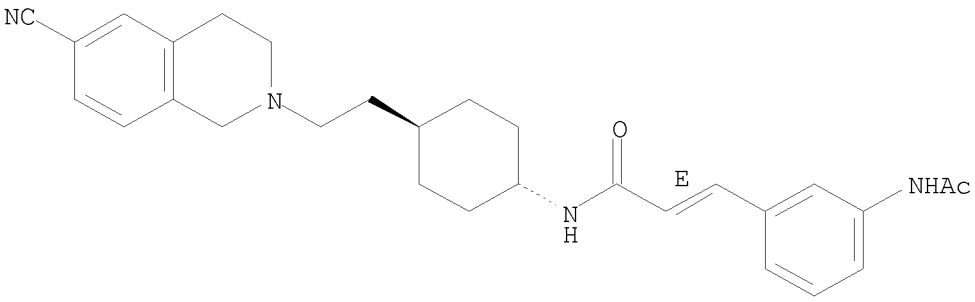
RN 215804-36-7 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-6-methyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-phenyl-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



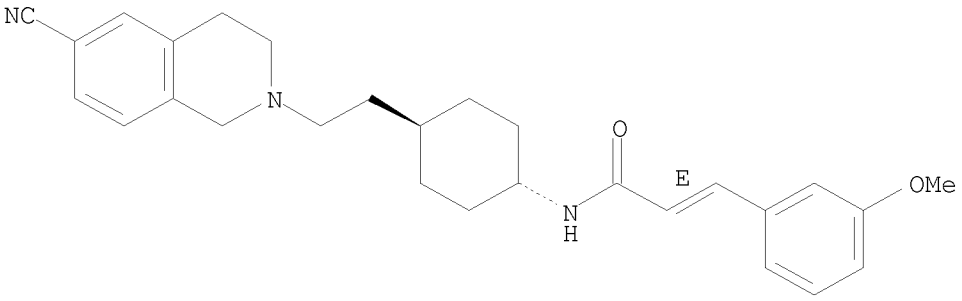
RN 215804-37-8 CAPLUS
CN 2-Propenamide, 3-[3-(acetylamino)phenyl]-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



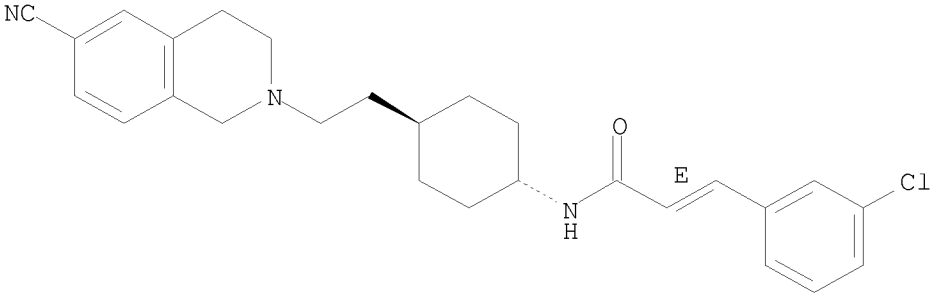
RN 215804-38-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(3-methoxyphenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



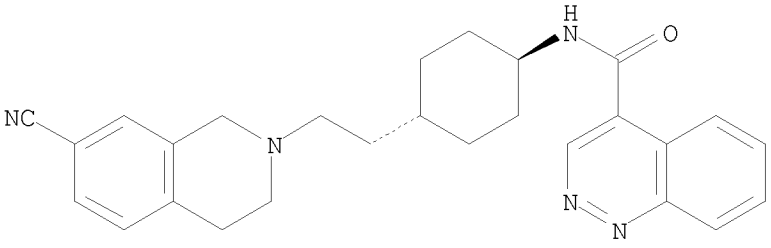
RN 215804-39-0 CAPLUS
CN 2-Propenamide, 3-(3-chlorophenyl)-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



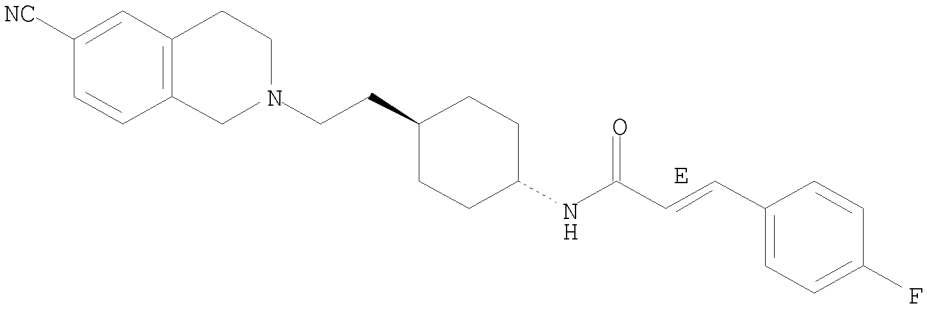
RN 215804-41-4 CAPLUS
CN 4-Cinnolinecarboxamide, N-[trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



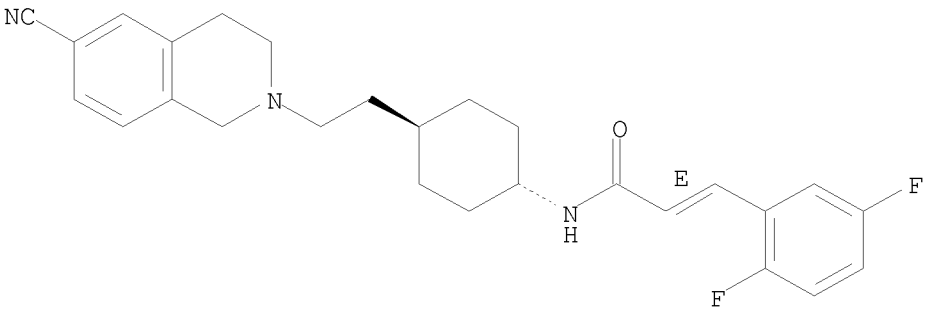
RN 215804-42-5 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(4-fluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



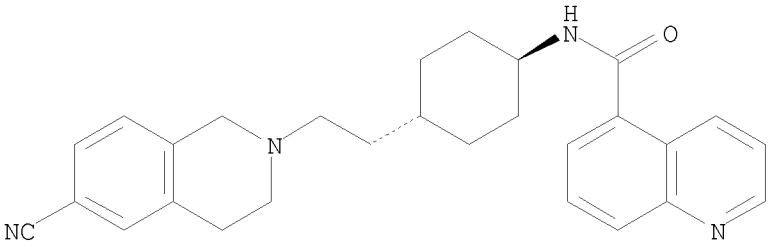
RN 215804-43-6 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2,5-difluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



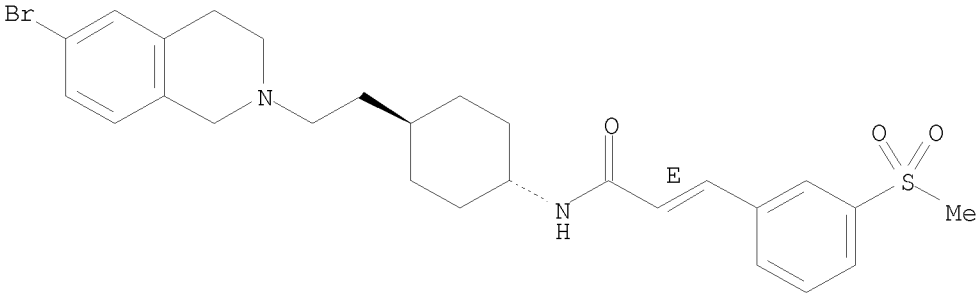
RN 215804-44-7 CAPLUS
CN 5-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 215804-45-8 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-bromo-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-[3-(methylsulfonyl)phenyl]-, (2E)- (CA INDEX NAME)

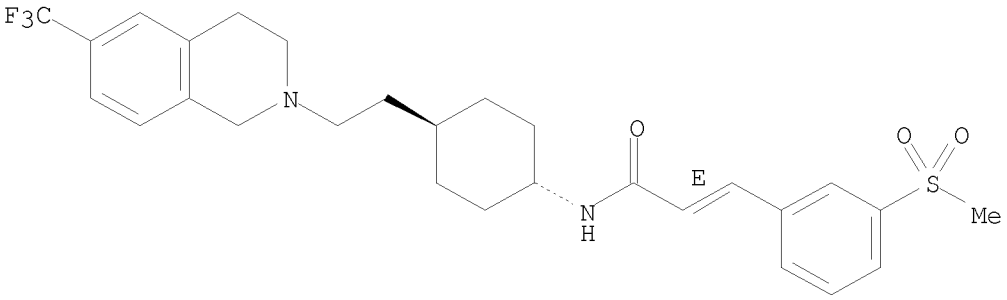
Relative stereochemistry.
Double bond geometry as shown.



RN 215804-46-9 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-[3,4-dihydro-6-(trifluoromethyl)-2(1H)-

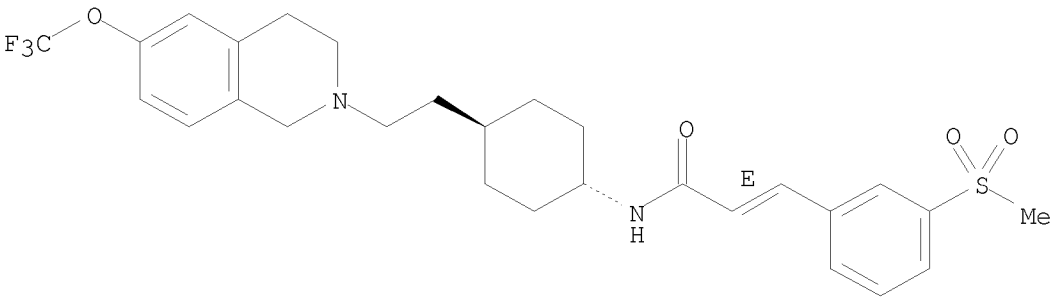
isoquinolinyl]ethyl]cyclohexyl]-3-[3-(methylsulfonyl)phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



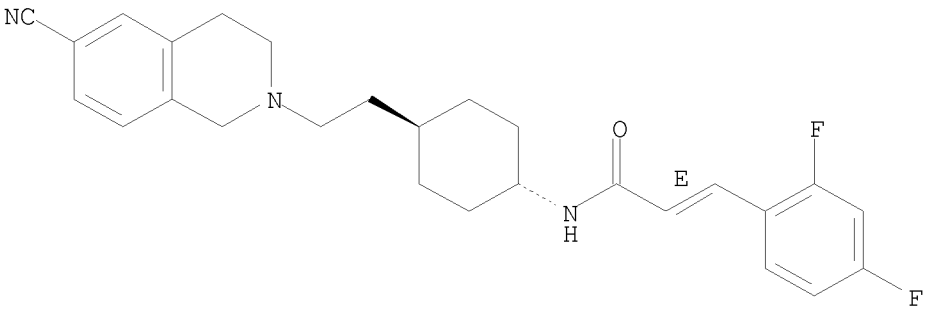
RN 215804-47-0 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-[3,4-dihydro-6-(trifluoromethoxy)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-3-[3-(methylsulfonyl)phenyl]-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



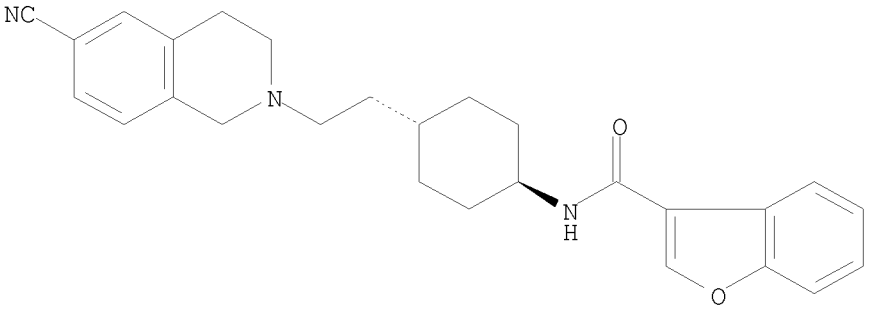
RN 215804-48-1 CAPLUS
CN 2-Propenamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-(2,4-difluorophenyl)-, (2E)- (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



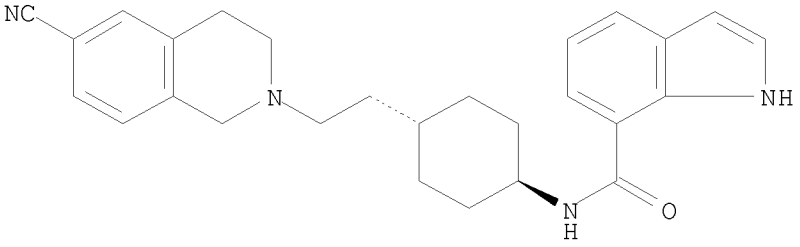
RN 215804-49-2 CAPLUS
CN 3-Benzofurancarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



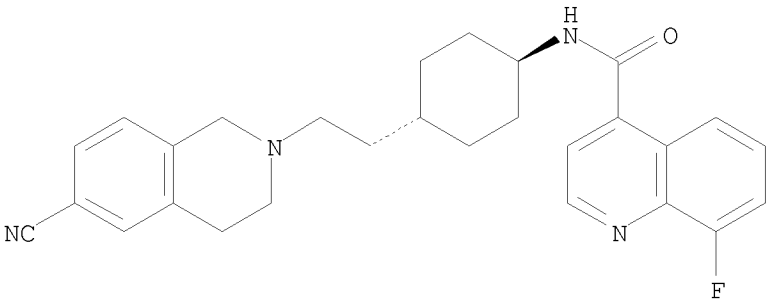
RN 215804-50-5 CAPLUS
CN 1H-Indole-7-carboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



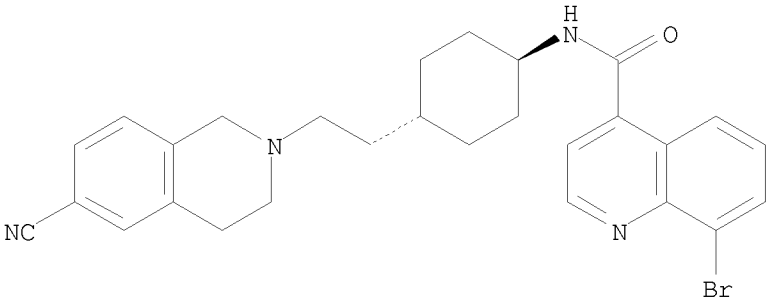
RN 215804-51-6 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-8-fluoro- (CA INDEX NAME)

Relative stereochemistry.



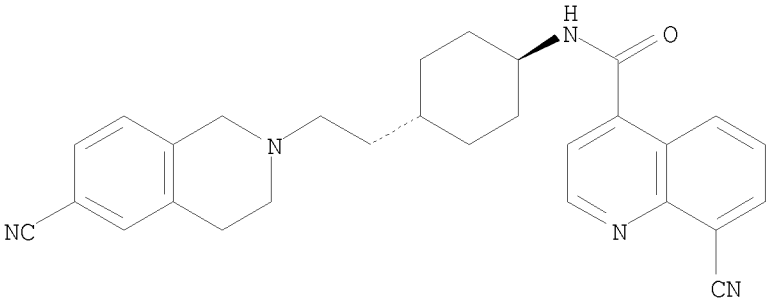
RN 215804-52-7 CAPLUS
CN 4-Quinolinecarboxamide, 8-bromo-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



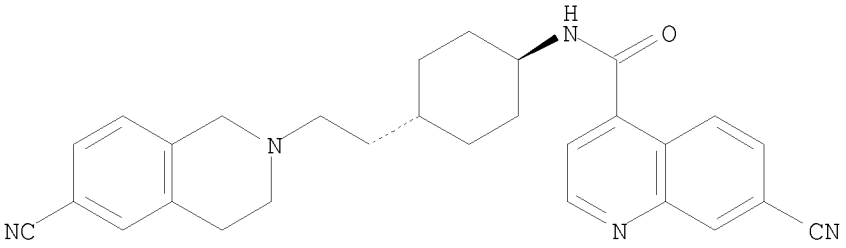
RN 215804-53-8 CAPLUS
CN 4-Quinolinecarboxamide, 8-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



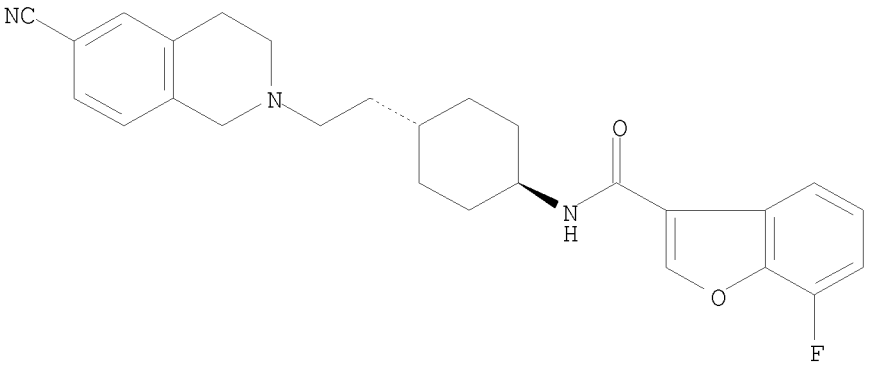
RN 215804-55-0 CAPLUS
CN 4-Quinolinecarboxamide, 7-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



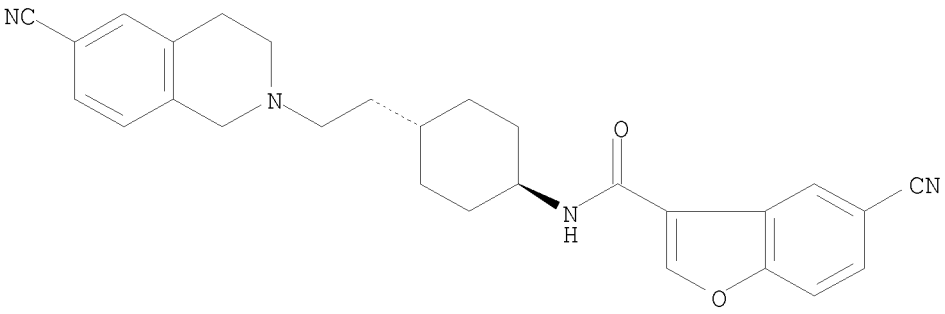
RN 215804-56-1 CAPLUS
CN 3-Benzofurancarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-7-fluoro- (CA INDEX NAME)

Relative stereochemistry.



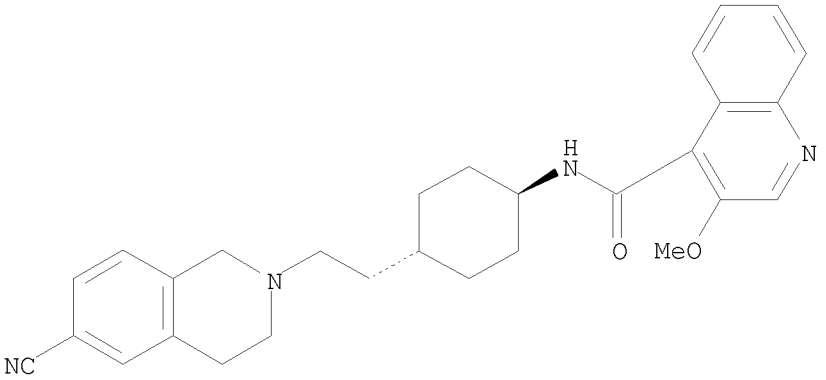
RN 215804-57-2 CAPLUS
CN 3-Benzofurancarboxamide, 5-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



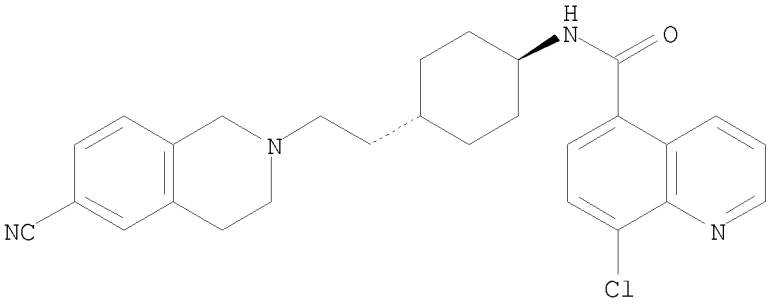
RN 215804-58-3 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-3-methoxy- (CA INDEX NAME)

Relative stereochemistry.



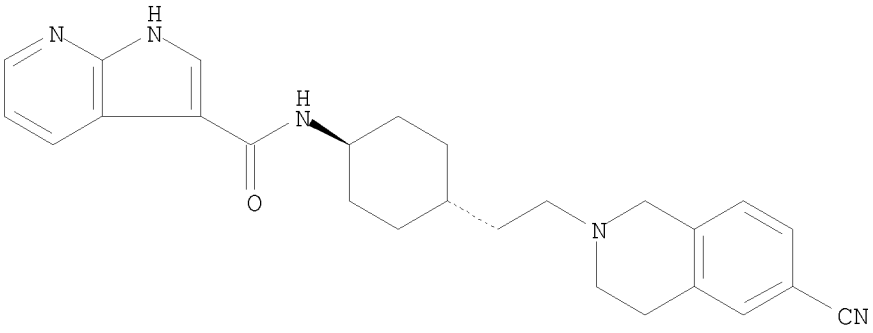
RN 215804-60-7 CAPLUS
CN 5-Quinolinecarboxamide, 8-chloro-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.



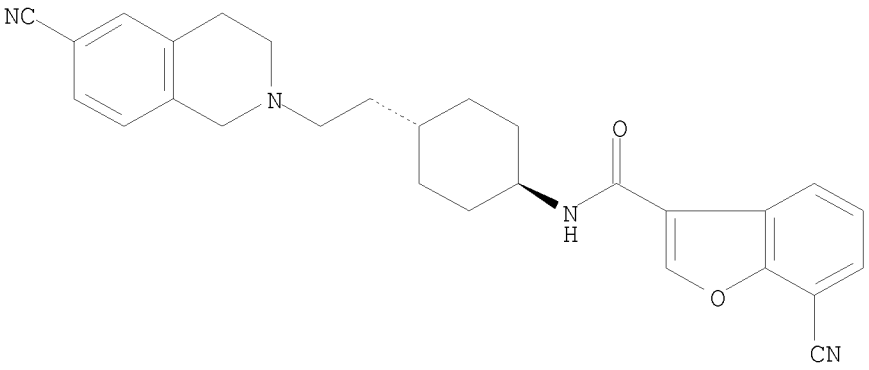
RN 215804-61-8 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine-3-carboxamide,
N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-
(CA INDEX NAME)

Relative stereochemistry.



RN 215804-62-9 CAPLUS
CN 3-Benzofurancarboxamide, 7-cyano-N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-
isoquinolinyl)ethyl]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

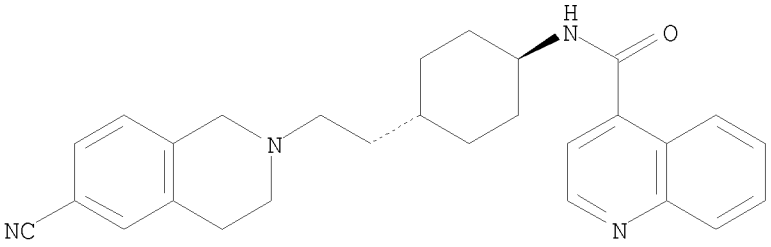


RN 215804-66-3 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-
isoquinolinyl)ethyl]cyclohexyl]-, methanesulfonate (1:1) (CA INDEX NAME)

CM 1

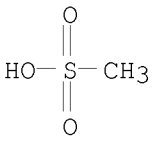
CRN 215803-78-4
CMF C28 H30 N4 O

Relative stereochemistry.



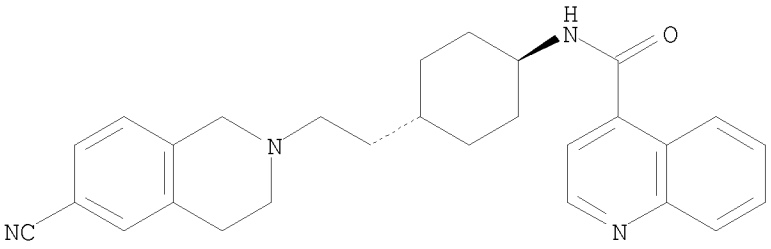
CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 215804-67-4 CAPLUS
CN 4-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, hydrochloride (1:1) (CA INDEX NAME)

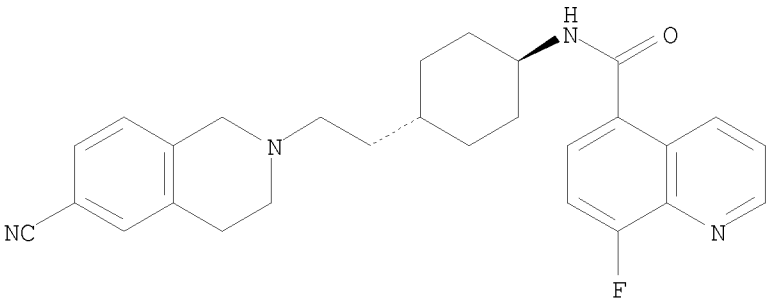
Relative stereochemistry.



● HCl

RN 215805-72-4 CAPLUS
CN 5-Quinolinecarboxamide, N-[trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-8-fluoro- (CA INDEX NAME)

Relative stereochemistry.

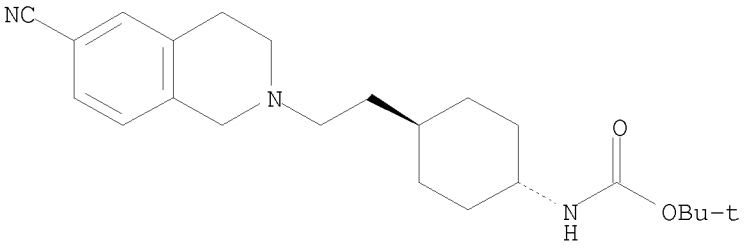


IT 215790-38-8P 215790-43-5P 215790-55-9P
215792-20-4P 215792-27-1P 215792-31-7P
215792-36-2P 215792-45-3P 215792-46-4P
215792-90-8P 215792-94-2P 215792-99-7P
215793-07-0P 215793-28-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-{2-(4-carboxamidocyclohexyl)ethyl]tetrahydroisoquinolines as dopamine D3 receptor ligands)

RN 215790-38-8 CAPLUS

CN Carbamic acid, [trans-4-[2-(6-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

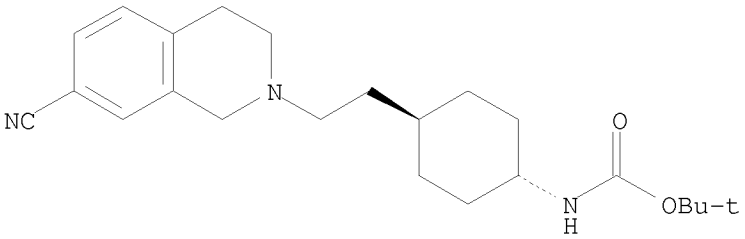
Relative stereochemistry.



RN 215790-43-5 CAPLUS

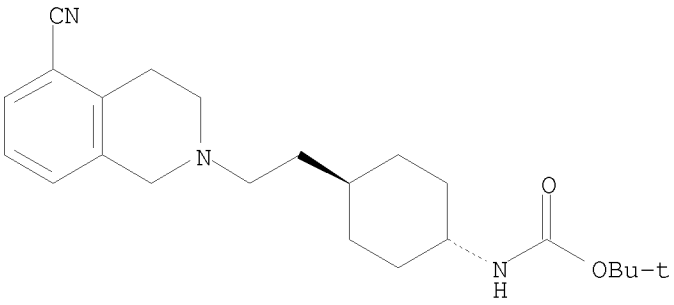
CN Carbamic acid, [trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



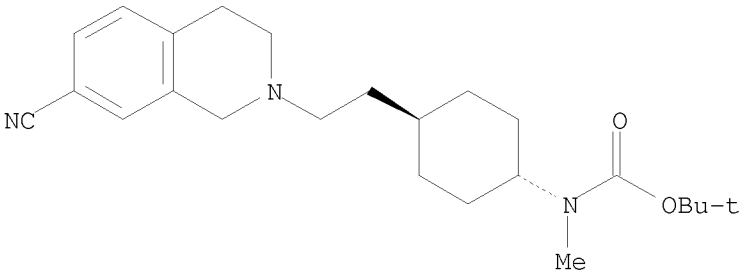
RN 215790-55-9 CAPLUS
CN Carbamic acid, [trans-4-[2-(5-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



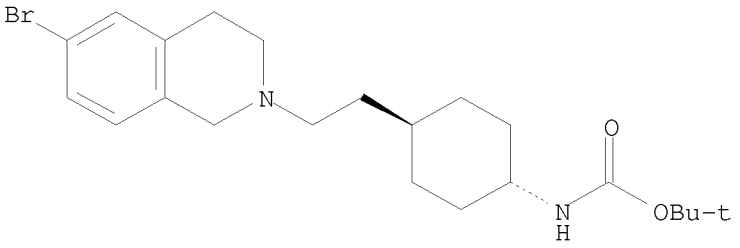
RN 215792-20-4 CAPLUS
CN Carbamic acid, [trans-4-[2-(7-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



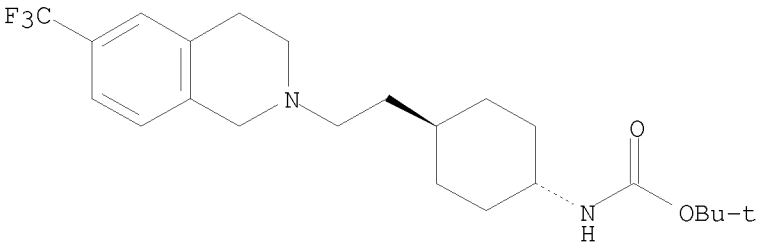
RN 215792-27-1 CAPLUS
CN Carbamic acid, [trans-4-[2-(6-bromo-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



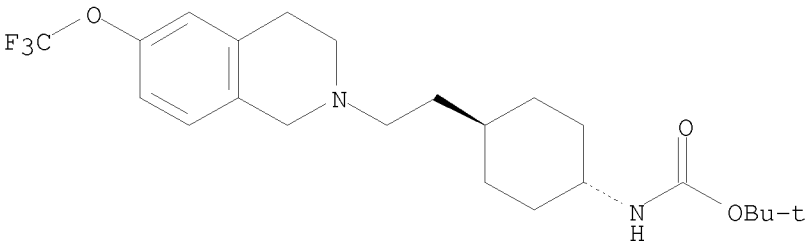
RN 215792-31-7 CAPLUS
CN Carbamic acid, [trans-4-[2-[3,4-dihydro-6-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 215792-36-2 CAPLUS
CN Carbamic acid, [trans-4-[2-[3,4-dihydro-6-(trifluoromethoxy)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

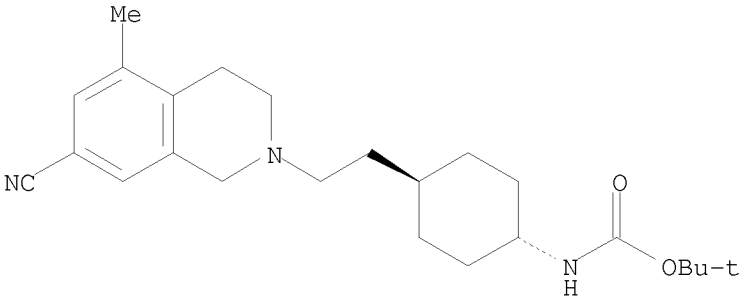
Relative stereochemistry.



RN 215792-45-3 CAPLUS
CN Carbamic acid, [trans-4-[2-(7-cyano-3,4-dihydro-5-methyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX

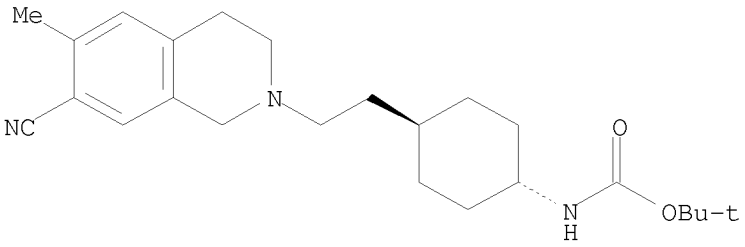
NAME)

Relative stereochemistry.



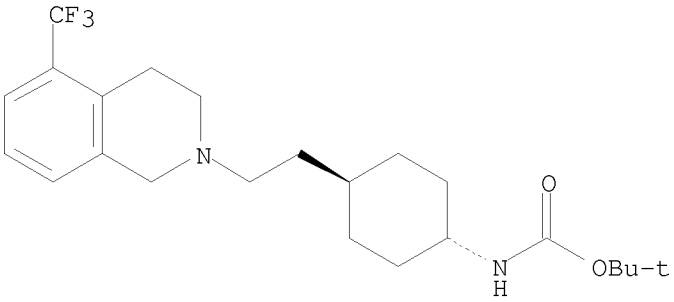
RN 215792-46-4 CAPLUS
CN Carbamic acid, [trans-4-[2-(7-cyano-3,4-dihydro-6-methyl-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



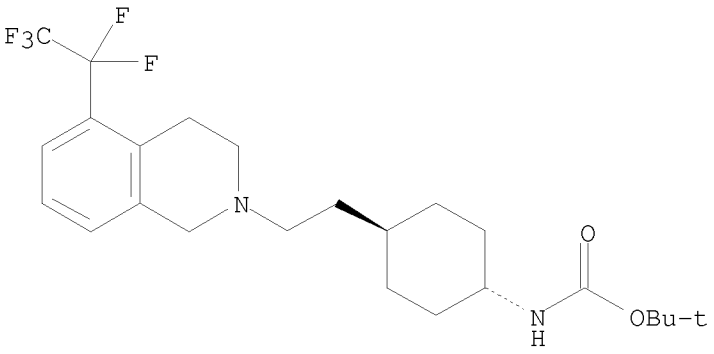
RN 215792-90-8 CAPLUS
CN Carbamic acid, [trans-4-[2-[3,4-dihydro-5-(trifluoromethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



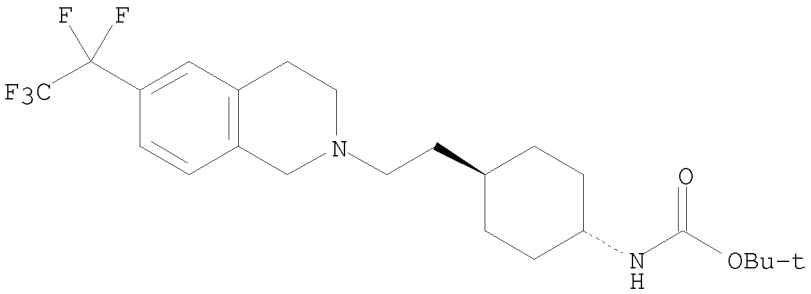
RN 215792-94-2 CAPLUS
CN Carbamic acid, [trans-4-[2-[3,4-dihydro-5-(pentafluoroethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



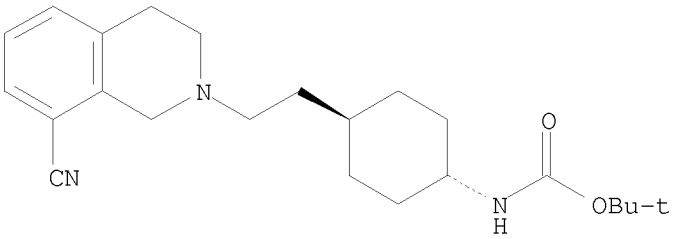
RN 215792-99-7 CAPLUS
CN Carbamic acid, [trans-4-[2-[3,4-dihydro-6-(pentafluoroethyl)-2(1H)-isoquinolinyl]ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



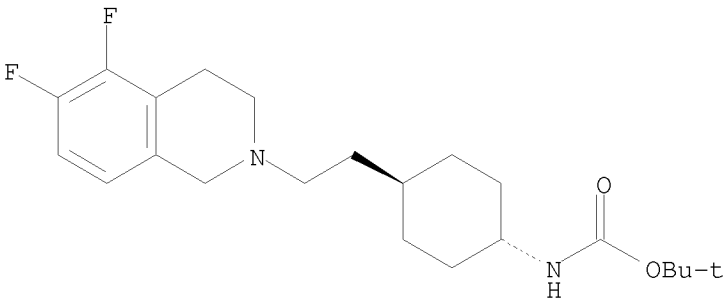
RN 215793-07-0 CAPLUS
CN Carbamic acid, [trans-4-[2-(8-cyano-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 215793-28-5 CAPLUS
CN Carbamic acid, [trans-4-[2-(5,6-difluoro-3,4-dihydro-2(1H)-isoquinolinyl)ethyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:717923 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 128:3692
ORIGINAL REFERENCE NO.: 128:799a,802a
TITLE: Fused imidazopyridine derivatives as antihyperlipidemic agents
INVENTOR(S): Takatani, Muneo; Shibouta, Yumiko; Sugiyama, Yasuo; Kawamoto, Tetsuji
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 457 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9740051	A1	19971030	WO 1997-JP1395	19970423 <--

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NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB,
GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN,
ML, MR, NE, SN, TD, TG

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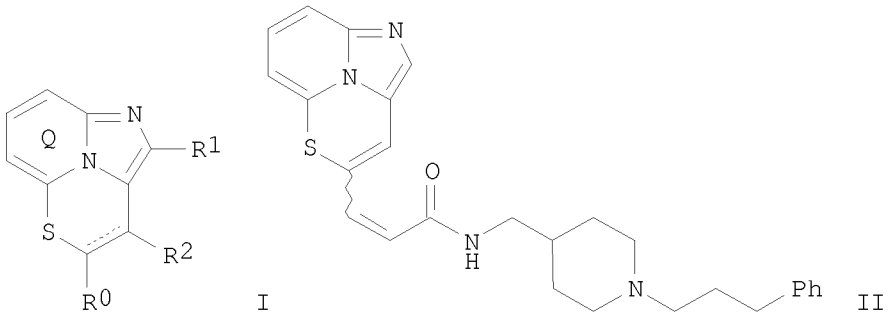
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
CN 1223659	A	19990721	CN 1997-193938		19970423 <--
US 6235731	B1	20010522	US 1998-155889		19981008 <--
PRIORITY APPLN. INFO.:			JP 1996-102303	A	19960424 <--
			JP 1996-330801	A	19961211 <--
			WO 1997-JP1395	W	19970423 <--

OTHER SOURCE(S): MARPAT 128:3692
GI

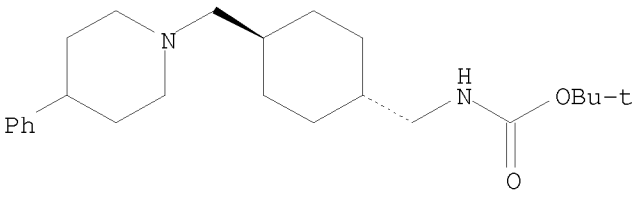


AB Novel compds. I [wherein ring Q is optionally substituted; one of R0, R1, and R2 = -Y0-Z0, and the others = H, halo, (un)substituted OH, (un)substituted hydrocarbyl, or acyl; Y0 = bond, (un)substituted bivalent hydrocarbon group; Z0 = basic group which may be bonded via O, N, CO, CS, SO2N(R3) (where R3 = H or (un)substituted hydrocarbyl), or S(O)n (where n = 0, 1, or 2); dotted line = optional pi bond] and salts thereof are disclosed. The compds. have excellent LDL receptor up-regulating, blood lipid-lowering, blood sugar-lowering, and diabetic complication-ameliorating activities. Examples include 178 synthetic examples, 79 reference examples, and biol. data for approx. 20 selected compds. For instance, Et 5-thia-1,8b-diazaacenaphthylene-4-carboxylate underwent a sequence of DIBAL reduction to an alc. (87%), oxidation to an aldehyde and Wittig-based homologation to an acrylic acid derivative (84%), amidation with 1-Boc-piperidin-4-ylmethylamine and deprotection (92%), N-alkylation with Ph(CH2)3Br (55%), and salification with methanolic HCl, to give the title compound II.2HCl. In hamsters, II.2HCl reduced non-HDL cholesterol to 62.3% of control, and triglycerides to 67.0% of control.

IT 198895-54-4P

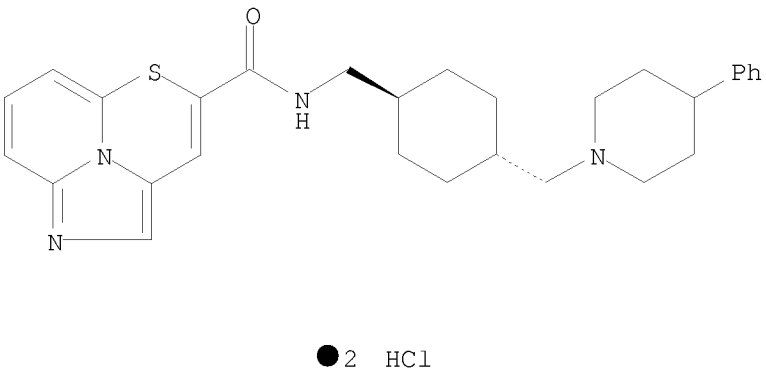
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fused imidazopyridine derivs. as antihyperlipidemic agents)
RN 198895-54-4 CAPLUS
CN Carbamic acid, [[4-[(4-phenyl-1-piperidinyl)methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



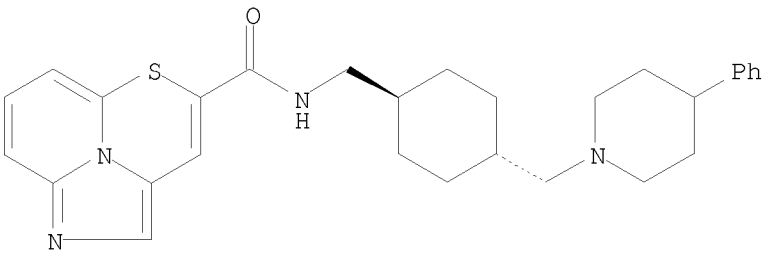
IT 198892-42-1P 198894-70-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused imidazopyridine derivs. as antihyperlipidemic agents)
RN 198892-42-1 CAPLUS
CN 5-Thia-1,8b-diazaacenaphthylene-4-carboxamide, N-[[4-[(4-phenyl-1-piperidinyl)methyl]cyclohexyl]methyl]-, dihydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 198894-70-1 CAPLUS
CN 5-Thia-1,8b-diazaacenaphthylene-4-carboxamide, N-[[4-[(4-phenyl-1-piperidinyl)methyl]cyclohexyl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 31 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:613831 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 127:278203
ORIGINAL REFERENCE NO.: 127:54337a,54340a
TITLE: Benzoxazinone and benzopyrimidinone piperidinyl tocolytic oxytocin receptor antagonists
INVENTOR(S): Bock, Mark G.; Evans, Ben E.; Williams, Peter D.; Freidinger, Roger M.; Pettibone, Douglas J.; Hobbs, Doug W.; Anderson, Paul S.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 140 pp., Cont.-in-part of U.S. Ser. No. 92,840, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5665719	A	19970909	US 1995-470693	19950606 <--
PRIORITY APPLN. INFO.:			US 1993-92840 B2	19930716 <--

OTHER SOURCE(S): MARPAT 127:278203
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

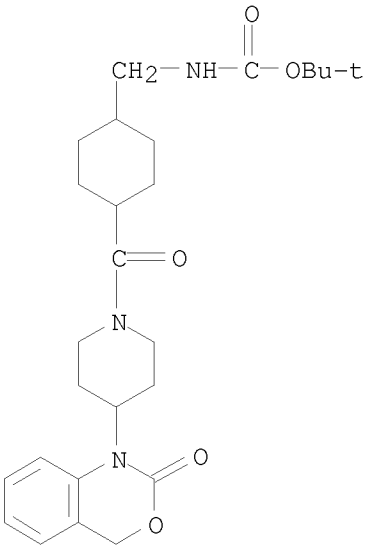
AB Compds. of formula I [X = O, NH, or NR8; Y = CH2, CHR8, or C(R8)2; R1 = camphor-10-yl, alkoxy, styryl, hydroxystyryl, furyl, (un)substituted thienyl, naphthyl, indolyl, tetrahydronaphthyl, (un)substituted pyridyl, pyrazinyl, (un)substituted cyclohexyl or Ph; R2 = H, alkoxy, alkyl, amino, alkylcarbonylamino, nitro, or halo; R3 = H, alkoxycarbonyl, cyano, or carbamoyl; and m = 0 or 1] and various analogs are disclosed. The compds. as useful as oxytocin (OT) and vasopressin receptor antagonists. Over 275 synthetic examples are given. For instance, Me 2,4-dihydroxybenzoate underwent Mitsunobu etherification with N-(tert-butoxycarbonyl)-4-piperidinol (51%), followed by O-methylation of the remaining hydroxyl (88%), saponification of the Me ester (95%), and coupling of the resultant acid with 1-(4-piperidinyl)-1,2-dihydro-4H-3,1-benzoxazin-

2-one (HCl salt) using EDC and HOBt (88%), to give title compound II [R = CO2Bu-tert]. The latter was deprotected with HCl in dioxane (93%) and acetylated with Ac2O (89%) to give title compound II [R = Ac]. The latter inhibited binding of [3H]-OT to rat uterine OT receptors in vitro with an IC50 of 47 nM.

IT 162043-68-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoxazinone and benzopyrimidinone derivs. as oxytocin and vasopressin receptor antagonists)

RN 162043-68-7 CAPLUS

CN Carbamic acid, [[4-[[4-(2-oxo-2H-3,1-benzoxazin-1(4H)-yl)-1-piperidinyl]carbonyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L18 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:466913 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 125:142726
ORIGINAL REFERENCE NO.: 125:26717a,26720a
TITLE: Muscarine antagonists
INVENTOR(S): Thompson, Wayne J.; Sugrue, Michael F.; Ransom, Richard W.; Mallorga, Pierre J.; Bell, Ian M.; Smith, Anthony M.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 125 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9613262	A1	19960509	WO 1995-US13710	19951024 <--
W: AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, US, UZ				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5574044	A	19961112	US 1994-329757	19941027 <--
US 5691323	A	19971125	US 1995-440153	19950512 <--
CA 2200468	A1	19960509	CA 1995-2200468	19951024 <--
AU 9539674	A	19960523	AU 1995-39674	19951024 <--
AU 701127	B2	19990121		
EP 786997	A1	19970806	EP 1995-937615	19951024 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 2002515008	T	20020521	JP 1996-514691	19951024 <--
PRIORITY APPLN. INFO.:			US 1994-329757 A2	19941027 <--
			US 1995-440153 A2	19950512 <--
			WO 1995-US13710 W	19951024 <--

OTHER SOURCE(S): CASREACT 125:142726; MARPAT 125:142726

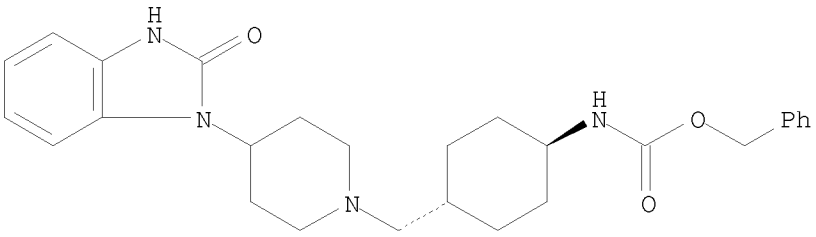
AB Compds., 1,3-dihydro-1-{1-[piperidin-4-yl]piperidin-4-yl}-2H-benzimidazol-2-ones and 1,3-dihydro-1-{4-amino-1-cyclohexyl}-2H-benzimidazol-2-ones and derivs. thereof, their preparation, method of use and pharmaceutical compns. are described. These compds. are endowed with antimuscarinic activity and are useful in the treatment and/or prevention of myopia (commonly known as nearsightedness).

IT 179322-84-0P 179322-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 179322-84-0 CAPLUS

CN Carbamic acid, [4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)-1-piperidinyl]methyl]cyclohexyl]-, phenylmethyl ester, trans- (9CI) (CA INDEX NAME)

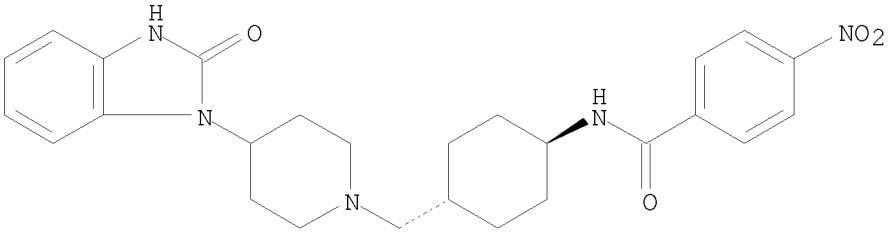
Relative stereochemistry.



RN 179322-94-2 CAPLUS

CN Benzamide, N-[4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)-1-piperidinyl]methyl]cyclohexyl]-4-nitro-, trans- (9CI) (CA INDEX NAME)

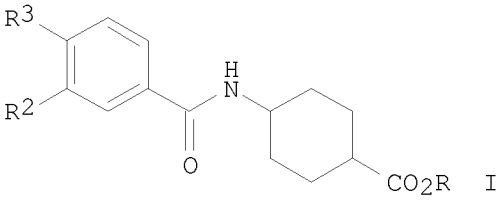
Relative stereochemistry.



L18 ANSWER 33 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:849158 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 123:256522
ORIGINAL REFERENCE NO.: 123:45879a,45882a
TITLE: Preparation of amide group-containing compounds as antithrombotics
INVENTOR(S): Himmelsbach, Frank; Linz, Guenter; Pieper, Helmut; Austel, Volkhard; Mueller, Thomas; Weisenberger, Johannes; Guth, Brian
PATENT ASSIGNEE(S): Dr. Karl Thomae GmbH, Germany
SOURCE: Ger. Offen., 46 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4326344	A1	19950209	DE 1993-4326344	19930805 <--
EP 638553	A1	19950215	EP 1994-111620	19940726 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CA 2129374	A1	19950206	CA 1994-2129374	19940803 <--
JP 07179424	A	19950718	JP 1994-183292	19940804 <--
PRIORITY APPLN. INFO.:			DE 1993-4326344 A	19930805 <--

OTHER SOURCE(S): CASREACT 123:256522; MARPAT 123:256522
GI



AB R1Z1Z2ZZ3Z4R4 [R1 = (un)substituted (di)azacycloalkyl, pyridyl; R4 = CO2H, alkoxycarbonyl, SO2H, tetrazolyl, etc.; Z = COZ5, Z5CO, Z5CONH, NHCOZ5, etc.; Z1 = bond, alk(en)ylene, O, S, NH, etc.; Z2 = (un)substituted phenylene, cycloalkylene, etc.; Z3 = alk(en)ylene, phenylene, etc.; Z4 =

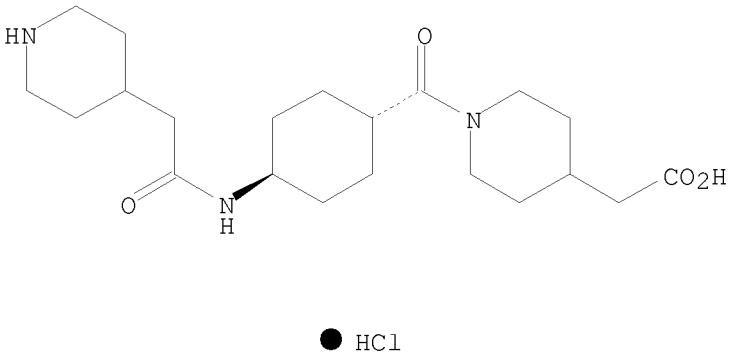
bond, OZ5, SO0-2Z5, NHZ5, etc.; Z5 = alkylene] were prepared Thus, quinuclidine was condensed with the ylide from 3-(Ph3P+H2C)C6H4CO2Me Br- and the reduced and saponified product condensed with Me trans-4-aminocyclohexanecarboxylate to give title compound trans-I.HCl (R = Me, R2 = 4-quinuclidinylethyl, R3 = H). Trans-I.HCl (R = R2 = H, R3 = 4-quinuclidinylmethoxy) had IC50 of 85nM against BIBU 52 binding at human thrombocytes in vitro.

IT 168891-16-5P 168891-18-7P 168891-21-2P
168891-51-8P 168891-53-0P 168891-55-2P
168891-94-9P 168891-95-0P 168891-97-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amide group-containing compds. as antithrombotics)

RN 168891-16-5 CAPLUS

CN 4-Piperidineacetic acid, 1-[[4-[(4-piperidinylacetyl)amino]cyclohexyl]carbonyl]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

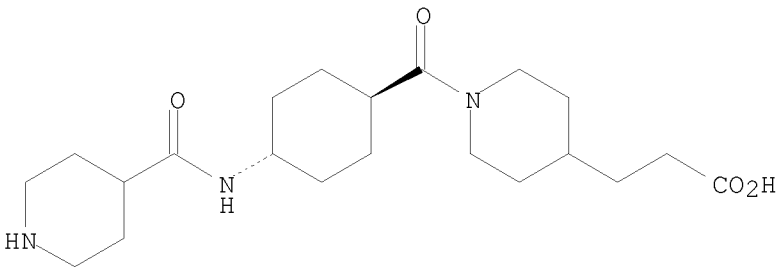
Relative stereochemistry.



RN 168891-18-7 CAPLUS

CN 4-Piperidinepropanoic acid, 1-[[4-[(4-piperidinylcarbonyl)amino]cyclohexyl]carbonyl]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

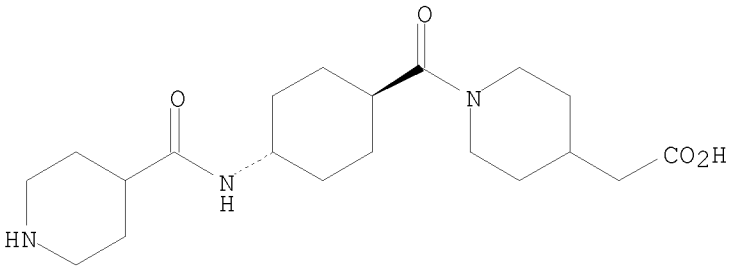
Relative stereochemistry.



● HCl

RN 168891-21-2 CAPLUS
CN 4-Piperidineacetic acid, 1-[[4-[(4-piperidinylcarbonyl)amino]cyclohexyl]carbonyl]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

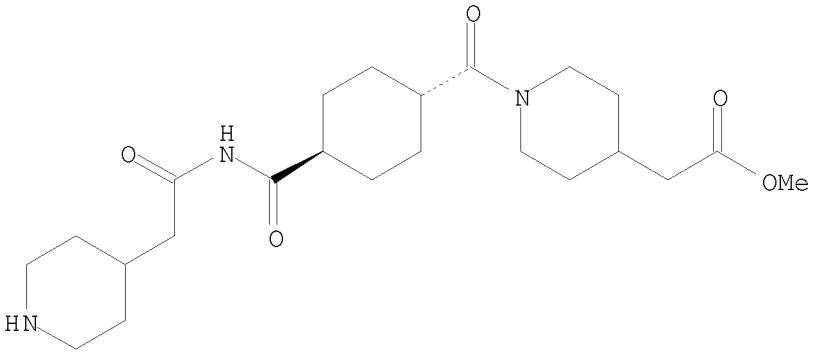
Relative stereochemistry.



● HCl

RN 168891-51-8 CAPLUS
CN 4-Piperidineacetic acid, 1-[[4-[[(4-piperidinylacetyl)amino]carbonyl]cyclohexyl]carbonyl]-, methyl ester, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



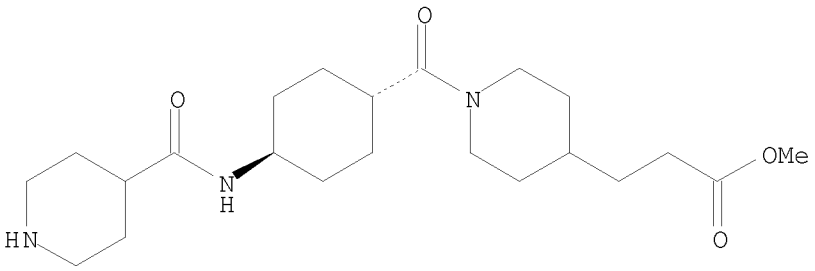
● HCl

RN 168891-53-0 CAPLUS
CN 4-Piperidinepropanoic acid, 1-[[4-[(4-piperidinylcarbonyl)amino]cyclohexyl]carbonyl]-, methyl ester, trans-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

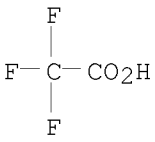
CRN 168891-52-9
CMF C22 H37 N3 O4

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

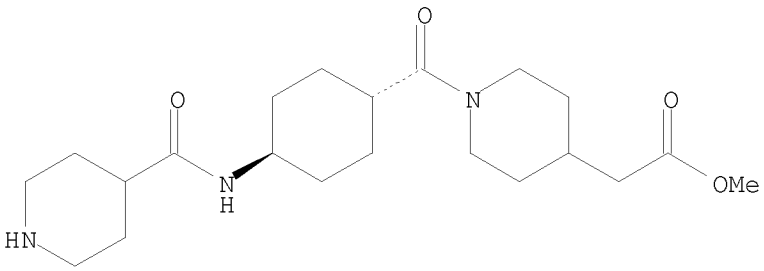


RN 168891-55-2 CAPLUS
CN 4-Piperidineacetic acid, 1-[[4-[(4-piperidinylcarbonyl)amino]cyclohexyl]carbonyl]-, methyl ester, trans-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

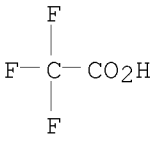
CRN 168891-54-1
CMF C21 H35 N3 O4

Relative stereochemistry.



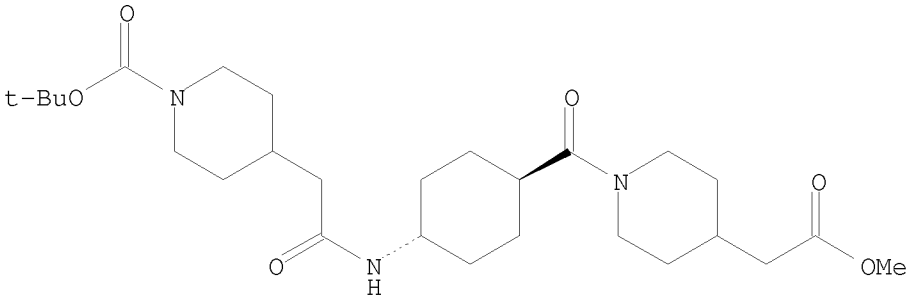
CM 2

CRN 76-05-1
CMF C2 H F3 O2



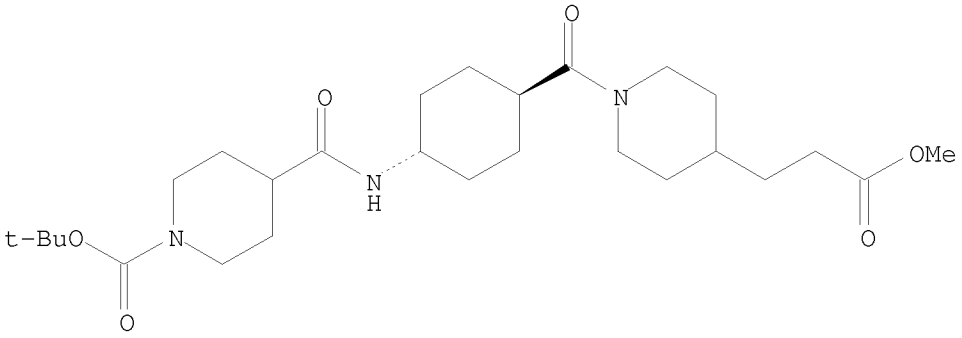
RN 168891-94-9 CAPLUS
CN 4-Piperidineacetic acid, 1-[[4-[[[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]acetyl]amino]cyclohexyl]carbonyl]-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



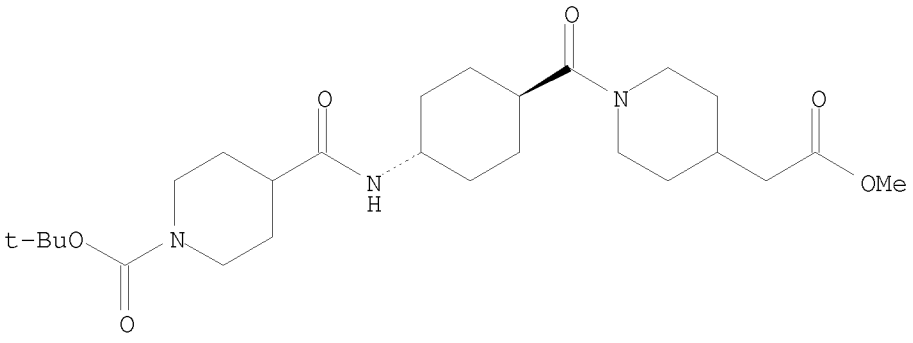
RN 168891-95-0 CAPLUS
CN 4-Piperidinepropanoic acid, 1-[[4-[[[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]carbonyl]amino]cyclohexyl]carbonyl]-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 168891-97-2 CAPLUS
CN 4-Piperidineacetic acid, 1-[[4-[[[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl]carbonyl]amino]cyclohexyl]carbonyl]-, methyl ester, trans- (9CI) (CA INDEX NAME)

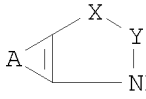
Relative stereochemistry.



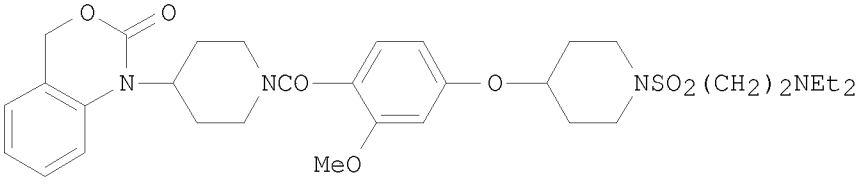
L18 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:470323 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 123:276051
ORIGINAL REFERENCE NO.: 123:49111a,49114a
TITLE: Benzoxazinone and benzopyrimidinone piperidinyl tocolytic oxytocin receptor antagonists
INVENTOR(S): Bock, Mark G.; Evans, Ben E.; Hobbs, Doug W.; Williams, Peter D.; Anderson, Paul S.; Freidinger, Roger M.; Pettibone, Douglas J.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 385 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9502405	A1	19950126	WO 1994-US7784	19940714 <--
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KE, KG, KR, KZ, LK, LT, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2166975	A1	19950126	CA 1994-2166975	19940714 <--
CA 2166975	C	20050405		
AU 9475132	A	19950213	AU 1994-75132	19940714 <--
AU 691829	B2	19980528		
EP 714299	A1	19960605	EP 1994-925092	19940714 <--
EP 714299	B1	20020424		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09500134	T	19970107	JP 1994-504656	19940714 <--
AT 216580	T	20020515	AT 1994-925092	19940714 <--
PRIORITY APPLN. INFO.:			US 1993-92840 A	19930716 <--
			WO 1994-US7784 W	19940714 <--

OTHER SOURCE(S): MARPAT 123:276051
GI



I



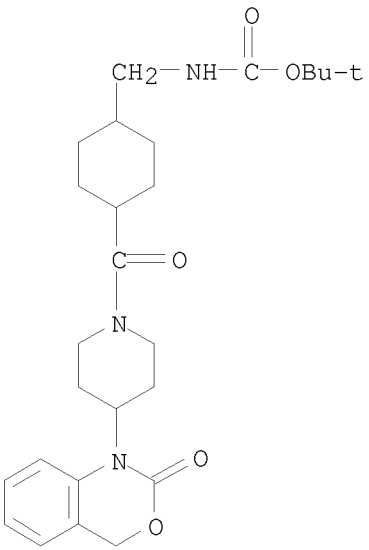
II

AB Fused N-containing heterocyclic ring system derivs. I [A completes a 5- or 6-membered carbocyclic or N- and/or S-containing heterocyclic ring; X = O, NH, (CH2)qO, CH2NH, OCH2, CH:CH, S, etc.; Y = CH2, C:O, C:S, C:NH, C:NMe; B = (substituted) N-containing heterocyclic or heterobicyclic ring; W = CH2, C:O, CO2, SO2, C(:NCH2Ph), etc.; R1 = (hetero)aryl, C1-5 alkoxy, camphor-10-yl] are useful as oxytocin and vasopressin receptor antagonists, e.g in treatment of preterm labor and dysmenorrhea and in stopping labor preparatory to cesarean delivery. Thus, in competitive radioligand binding assays on rat uterus membrane prepns., high-affinity binding of oxytocin-3H was inhibited by 1-[1-[4-[1-[(diethylaminoethyl)sulfonyl]-4-piperidinyloxy]-2-methoxybenzoyl]piperidin-4-yl]-1,2-dihydro-4H-3,1-benzoxazin-2-one (II) with an IC50 of 23 nM. II was prepared in 7 steps from Me 2,4-dihydroxybenzoate, N-tert-butyloxy-4-piperidinol, 1-(4-piperidinyl)-1,2-dihydro-4H-3,1-benzoxazin-2-one-HCl (preparation given), ClCH2CH2SO2Cl, and HNEt2. Preparation of 277 compds. of formula I is described.

IT 162043-68-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzoxazinone and benzopyrimidinone piperidinyl tocolytic oxytocin receptor antagonists)

RN 162043-68-7 CAPLUS

CN Carbamic acid, [[4-[[4-(2-oxo-2H-3,1-benzoxazin-1(4H)-yl)-1-piperidinyl]carbonyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

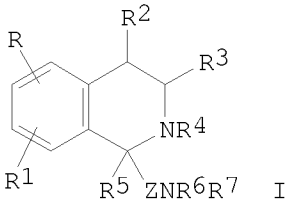


L18 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:89195 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 98:89195

ORIGINAL REFERENCE NO.: 98:13611a,13614a
TITLE: Isoquinoline derivatives
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57139066	A	19820827	JP 1981-24812	19810220 <--

PRIORITY APPLN. INFO.: JP 1981-24812 19810220 <--
OTHER SOURCE(S): CASREACT 98:89195
GI



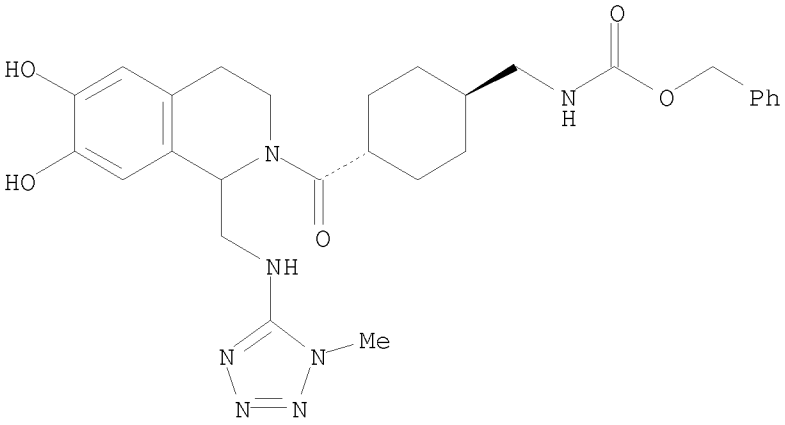
I

AB Thirty-seven isoquinoline derivs. I (R, R1 = H, OH, acyloxy, alkoxy; R2, R3 = H; R2 and R3 may be a bond; R4 = H, acyl; R5 = H; R4 and R5 may be a bond; R6 = H, alkyl; R7 = alkyl-substituted 5-membered N heterocyclic; Z = alkylene) were prepared by, e.g., reaction of RR1C6H3CH2CH2NH2 (II) with R6R7NZCHO (III). Antiulcer test data of I were shown. Thus, stirring a mixture of 2.15 g (1-methyl-1H-tetrazol-5-yl)aminoacetaldehyde di-Et acetal and 3 mL MeI in DMF with 0.57 g 65% NaH 2 h at 5° gave 2.18 g III di-Et acetal (R6 = Me, R7 = 1-methyl-1H-tetrazol-5-yl, Z = CH2) (IV). A mixture of 2.84 g IV, 4.6 g II.HCl (R ,R1 = 3-,4-OH), and 0.9 mL concentrated HCl in aqueous EtOH was stirred for 5 h at 90° to give 2.3 g I.HCl (R,R1 = 3-, 4-OH, R2 = R3 = R4 = R5 = H, R6 = Me, R7 = 1-methyl-1H-tetrazol-5-yl, Z = CH2).

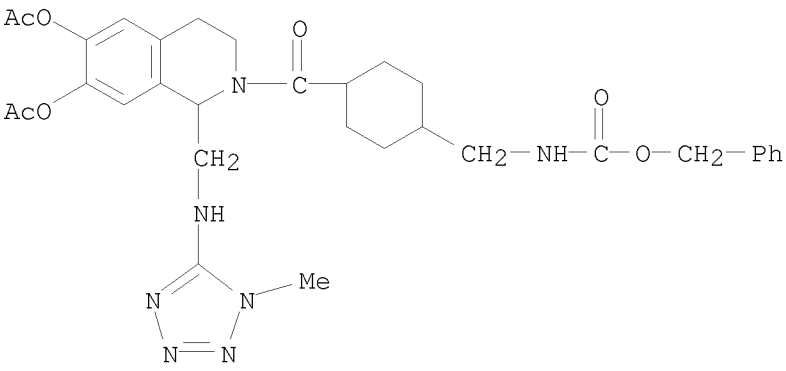
IT 84641-15-6P 84641-34-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiulcer activity of)

RN 84641-15-6 CAPLUS
CN Carbamic acid, [[4-[[3,4-dihydro-6,7-dihydroxy-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-2(1H)-isoquinolinyl]carbonyl]cyclohexyl]methyl]-, phenylmethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 84641-34-9 CAPLUS
CN Carbamic acid, [[4-[[6,7-bis(acetyloxy)-3,4-dihydro-1-[[(1-methyl-1H-tetrazol-5-yl)amino]methyl]-2(1H)-isoquinolinyl]carbonyl]cyclohexyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



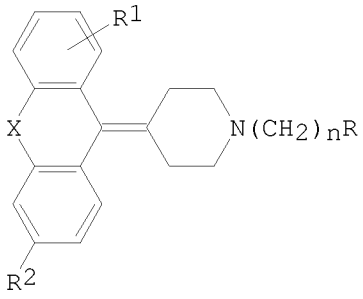
L18 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:408028 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 93:8028
ORIGINAL REFERENCE NO.: 93:1471a,1474a
TITLE: Xanthone and thioxanthone derivatives and compositions containing them
INVENTOR(S): Lassen, Niels; Bogeso, Klaus Peter; Hansen, Peter Bregnedal; Buus, Jorn Lasse Martin; Bigler, Allan Johan
PATENT ASSIGNEE(S): Kefalas A/S, Den.
SOURCE: Eur. Pat. Appl., 51 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 5607	A1	19791128	EP 1979-300778	19790504 <--
EP 5607	B1	19831026		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
US 4285956	A	19810825	US 1979-35735	19790503 <--
AT 5141	T	19831115	AT 1979-300778	19790504 <--
DK 7901901	A	19791113	DK 1979-1901	19790509 <--
ZA 7902250	A	19800827	ZA 1979-2250	19790509 <--
FI 7901503	A	19791113	FI 1979-1503	19790510 <--
AU 7946941	A	19791115	AU 1979-46941	19790510 <--
AU 522926	B2	19820701		
NO 7901592	A	19791113	NO 1979-1592	19790511 <--
NO 150837	B	19840917		
NO 150837	C	19850109		
CA 1127648	A1	19820713	CA 1979-327464	19790511 <--
JP 54154772	A	19791206	JP 1979-57640	19790512 <--
US 4275209	A	19810623	US 1979-106353	19791221 <--
US 4309429	A	19820105	US 1979-105985	19791221 <--

PRIORITY APPLN. INFO.: GB 1978-19310 19780512 <--
US 1979-35735 A3 19790503 <--
EP 1979-300778 A 19790504 <--

OTHER SOURCE(S): MARPAT 93:8028
GI

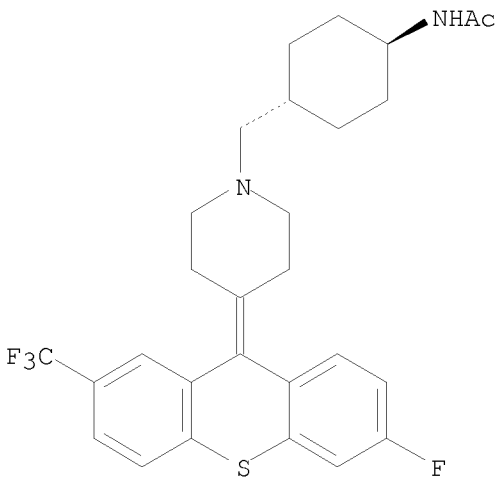


I

AB The neuroleptic compds. I (X = O, S; R = substituted cycloalkyl, optionally substituted heterocycle containing O and/or N; R1 = halogen, alkyl, alkoxy, SMe, SO2Me, SO2NMe2, CF3, Ac; R2 = H, F, Me; n = 0-3) were prepared Thus Grignard reaction of 2-trifluoromethyl-6-fluoro-9-thioxanthone with 4-chloro-1-methylpiperidine and dehydration of the alc. gave I (R = H, R1 = 2-CF3, R2 = F, X = S, n = 1), which was treated with ClCO2CH2CCl3 and decarboxylated to give I (X = S, R = H, R1 = 2-CF3, R2 = F, n = 0). This was acylated with trans-4-acetoxycyclohexanecarbonyl chloride, followed by LiAlH4 reduction to give I (X = S, R = trans-4-hydroxycyclohexyl, R1 = 2-CF3, R2 = F, n = 1; II). II had an amphetamine antagonist ED50 of 0.32 mg/kg i.p. in rats.

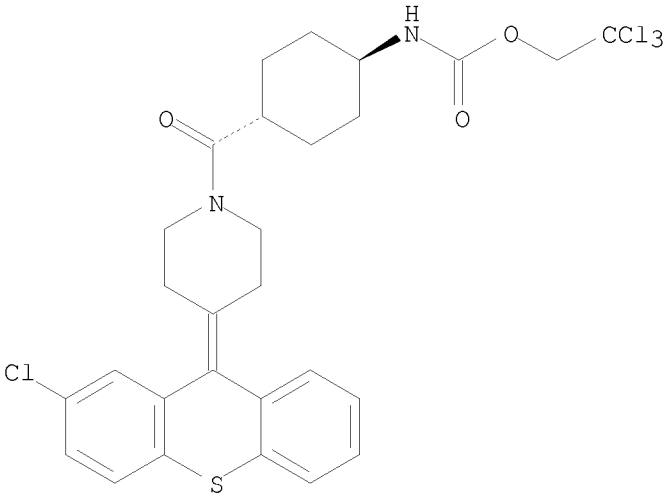
IT 73847-33-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and neuroleptic activity of)
RN 73847-33-3 CAPLUS
CN Acetamide, N-[4-[[4-[6-fluoro-2-(trifluoromethyl)-9H-thioxanthen-9-ylidene]-1-piperidinyl]methyl]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 73847-29-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 73847-29-7 CAPLUS
CN Carbamic acid, [4-[[4-(2-chloro-9H-thioxanthen-9-ylidene)-1-piperidinyl]carbonyl]cyclohexyl]-, 2,2,2-trichloroethyl ester, trans- (9CI) (CA INDEX NAME)

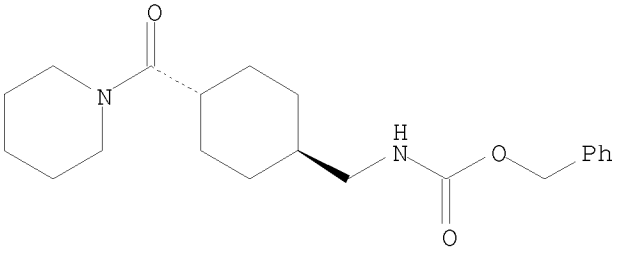
Relative stereochemistry.



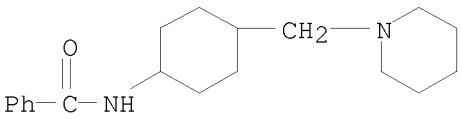
L18 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:400156 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 77:156
ORIGINAL REFERENCE NO.: 77:23a,26a
TITLE: Medicinal chemical studies on antiplasmin drugs. 4. Chemical modification of trans-4-aminomethylcyclohexanecarboxylic acid and its effect on antiplasmin activity
AUTHOR(S): Okano, Atsuji; Inaoko, Masato; Funabashi, Shoichi; Iwamoto, Masahiro; Isoda, Sumiro; Moroi, Reimei; Abiko, Yasushi; Hirata, Miyoshi
CORPORATE SOURCE: Res. Lab., Daiichi Seiyaku Co., Ltd., Tokyo, Japan
SOURCE: Journal of Medicinal Chemistry (1972), 15(3), 247-55
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of N-substituted derivs., amides, and esters of trans-4-aminomethylcyclohexanecarboxylic acid (I) [1197-18-8], prepared by known methods starting with I, was evaluated for antiplasmin activity in the caseinolytic and fibrinolytic reaction, using I, benzyl trans-4-aminomethylcyclohexanecarboxylate (II) [12565-25-2] or phenyl trans-4-aminomethylcyclohexanecarboxylate (III) [33445-24-8] as reference stds. The antiplasmin activity of I alkyl esters was superior to that of I in caseinolysis and unsatd. alkyl esters having a double or triple bond at the β-position of the alkoxy group were more potent than saturated alkyl esters. The potency of II relative to I was 41.8 and 1.6 in caseinolysis and fibrinolysis, resp. Conversion of the benzyl moiety into phenyl resulted in increased antiplasmin activity; e.g., III activity relative to I was increased 32 times in fibrinolysis. Generally, para phenyl substituents increased activity, meta substituents decreased activity to less than the corresponding para substituted compds, and ortho substitution decreased activity. P-carboxyethylphenyl trans-4-aminomethylcyclohexanecarboxylate (IV) [34675-84-8] was considered the most promising compound on the basis of antiplasmin activity, solubility, and

stability in H2O.
IT 38688-34-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38688-34-5 CAPLUS
CN Carbamic acid, [[4-(1-piperidinylcarbonyl)cyclohexyl]methyl]-, phenylmethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L18 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1955:17187 CAPLUS <<LOGINID::20081022>>
DOCUMENT NUMBER: 49:17187
ORIGINAL REFERENCE NO.: 49:3403e-g
TITLE: Local anesthetic action of certain amides
AUTHOR(S): Rose, Charles L.; Rawlings, Davis V.
CORPORATE SOURCE: Lilly Research Lab. Indianapolis, IN
SOURCE: Journal of Laboratory and Clinical Medicine (1954), 44, 571-81
CODEN: JLCMAK; ISSN: 0022-2143
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Twenty-five amides of 3-dialkylaminopropylamine of the generic formula RCONHR'CHCHR''CHR'''N(R'''')2 where R, R', and R'''' may be aryl or alkyl and R'' and R''' may be H or alkyl were tested. Duration of anesthesia was determined in the guinea-pig eye and intracutaneously in the same animal. Irritation was estimated on rabbit skin. Toxicity was determined in mice. 1-Benzamido-1-phenyl-3-piperidino propane-HCl was stable and active topically, intradermally, and intrathecally. It was nonirritating and only moderately toxic. α-1-Benzamido-2-methyl-1-phenyl-3-piperidinopropane-HCl was long acting on topical application and when given intradermally or intrathecally.
IT 857489-16-8, Benzamide, N-(4-piperidinomethylcyclohexyl)-
(α- and β-forms, anesthetic (local) action of)
RN 857489-16-8 CAPLUS
CN Benzamide, N-[4-(1-piperidinylmethyl)cyclohexyl]- (CA INDEX NAME)



(α- and β-forms, local anesthetic action of

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